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                  SEL RN

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L5                STR L3
L6              3 S L5
L7                STR L5
L8              3 S L7
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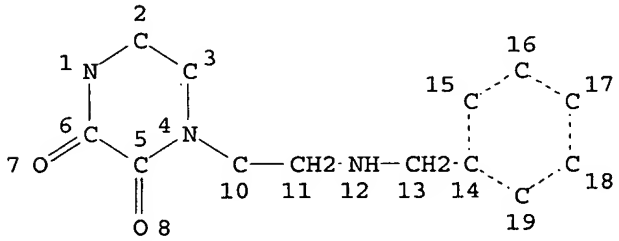


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NUMBER OF NODES IS  18

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L10 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:474920 HCAPLUS
DOCUMENT NUMBER: 143:19969
TITLE: Peptidyl and nonpeptidyl compounds for derepression of IAP-inhibited caspase and therapeutic and drug screening uses
INVENTOR(S): Reed, John C.; Houghten, Richard A.; Nefzi, Adel; Ostresh, John M.; Pinilla, Clemencia; Welsh, Kate
PATENT ASSIGNEE(S): The Burnham Institute, USA; Torrey Pines Institute for Molecular Studies
SOURCE: U.S. Pat. Appl. Publ., 182 pp., Cont.-in-part of U.S. Ser. No. 302,811.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

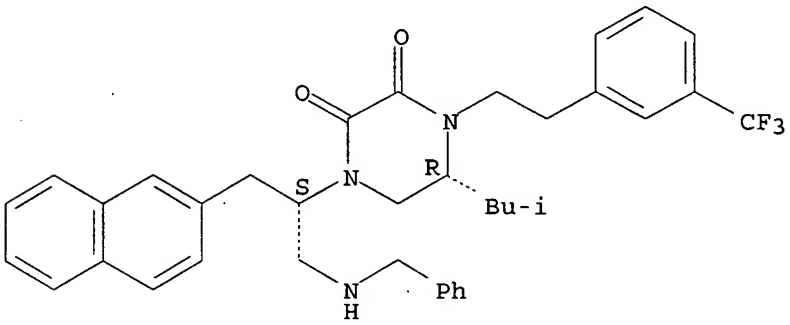
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2005119176	A1	20050602	US 2003-748128		2003 1224
US 2003180805	A1	20030925	US 2002-302811		2002 1121
US 6911426	B2	20050628			
US 2005159359	A1	20050721	US 2004-21517		2004 1223
PRIORITY APPLN. INFO.:			US 2001-331957P	P	2001 1121
			US 2002-302811	A2	2002 1121

AB The invention provides isolated agents having a core peptidyl or nonpeptidyl (e.g., urea derivative, diketopiperazine derivative) structure, wherein the agent derepresses an IAP-inhibited caspase. The invention also provides a method of derepressing an IAP-inhibited caspase. The method consists of contacting an IAP-inhibited caspase with an effective amount of an agent to derepress an IAP-inhibited caspase. The methods of the invention can be used for promoting apoptosis in a cell and for reducing the severity of a pathol. (e.g., cancer) characterized by reduced levels of apoptosis. Methods for identifying agents that derepress an IAP-inhibited caspase are also provided.
IT **537051-58-4 537051-59-5 537053-07-9 537053-08-0 537053-09-1 537053-10-4 537053-11-5 537053-12-6 537053-13-7**

537053-14-8 537053-15-9 537053-16-0
537053-17-1 537053-18-2 537053-19-3
537053-20-6 537053-21-7 537053-22-8
537053-23-9 537053-24-0 537053-25-1
537053-26-2 537053-27-3 537053-28-4
537053-29-5 537053-30-8 537053-31-9
537053-32-0 537053-33-1 540529-39-3
540529-41-7 540529-43-9 540529-46-2
540529-48-4 540529-50-8 852819-52-4
(peptidyl and nonpeptidyl compds. for derepression of IAP-inhibited caspase and therapeutic and drug screening uses)

RN 537051-58-4 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537051-59-5 HCAPLUS
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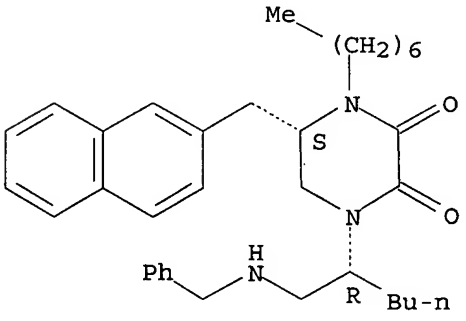
Absolute stereochemistry.



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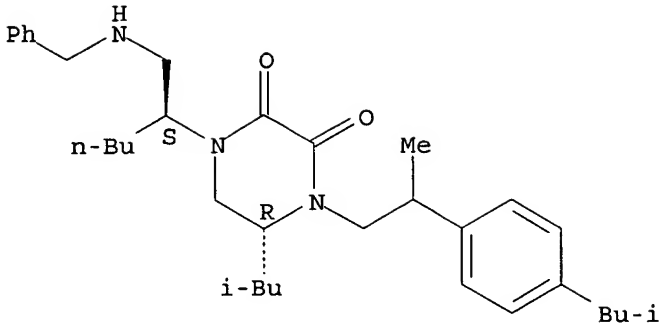
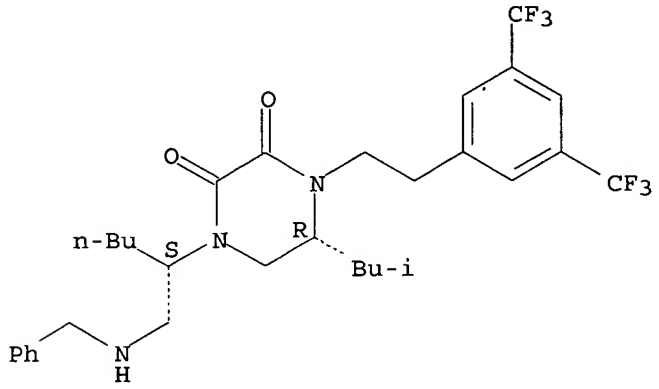
Absolute stereochemistry.



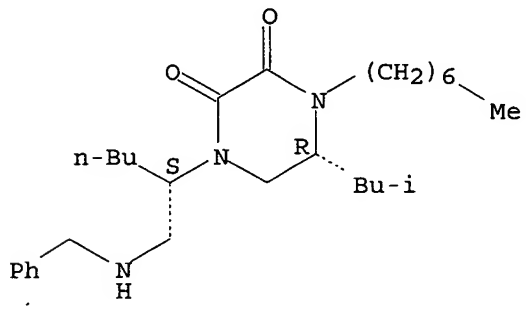
RN 537053-08-0 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-09-1 HCAPLUS
CN 2,3-Piperazinedione, 4-heptyl-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

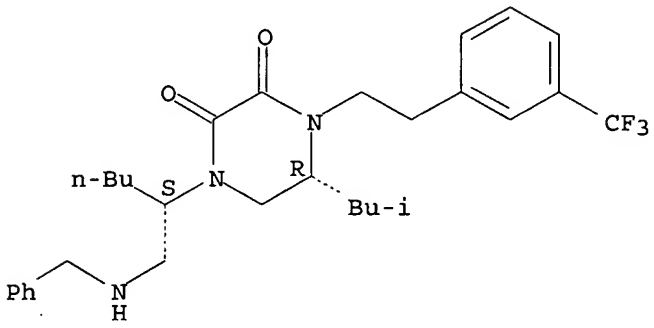
Absolute stereochemistry.



RN 537053-10-4 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-

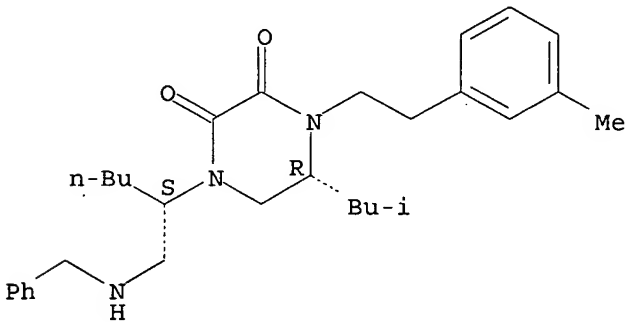
(trifluoromethyl)phenyl]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



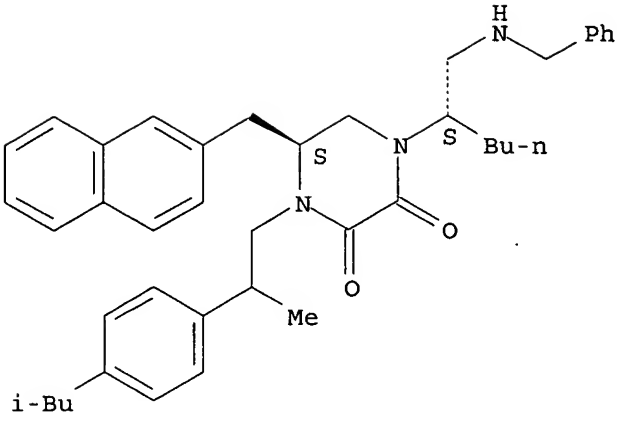
RN 537053-11-5 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



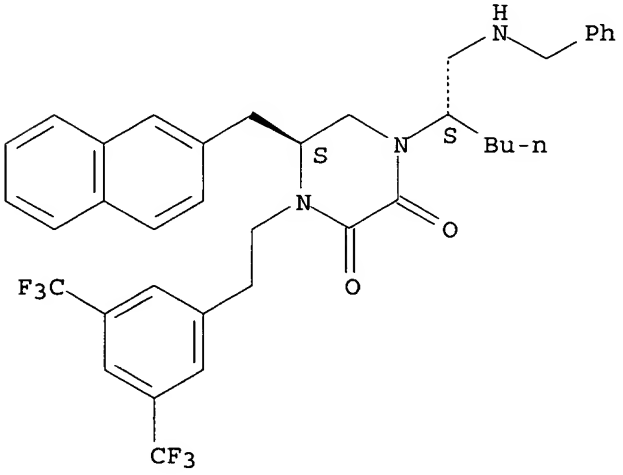
RN 537053-12-6 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[4-(2-methylpropyl)phenyl]propyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



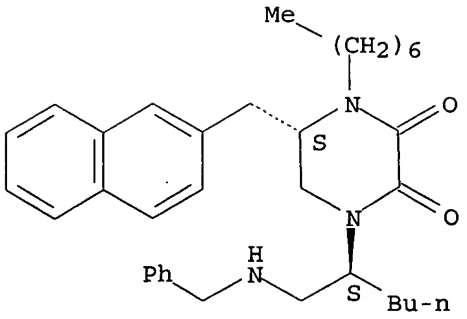
RN 537053-13-7 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



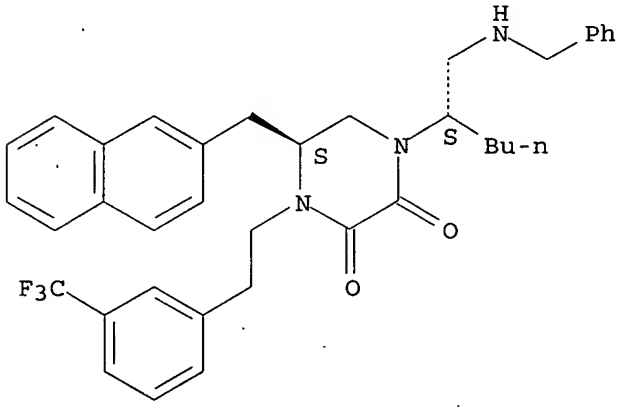
RN 537053-14-8 HCAPLUS
CN 2,3-Piperazinedione, 4-heptyl-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



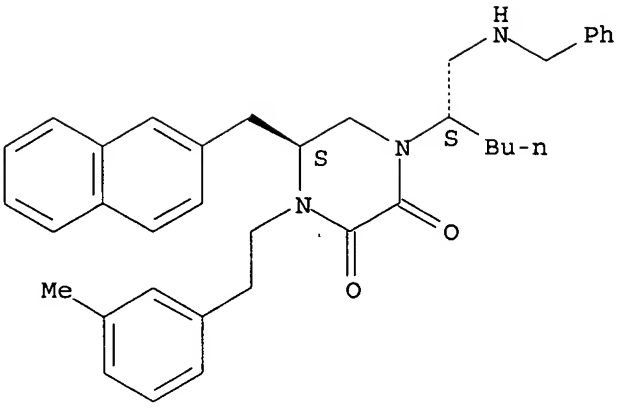
RN 537053-15-9 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



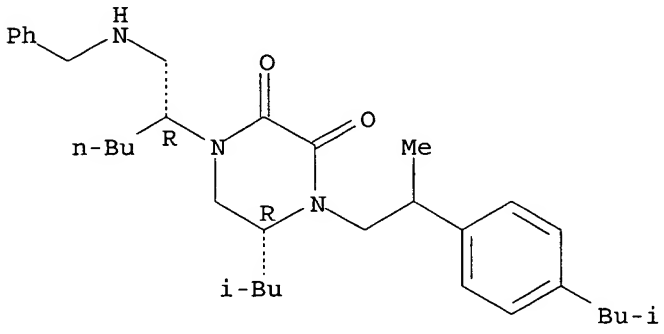
RN 537053-16-0 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



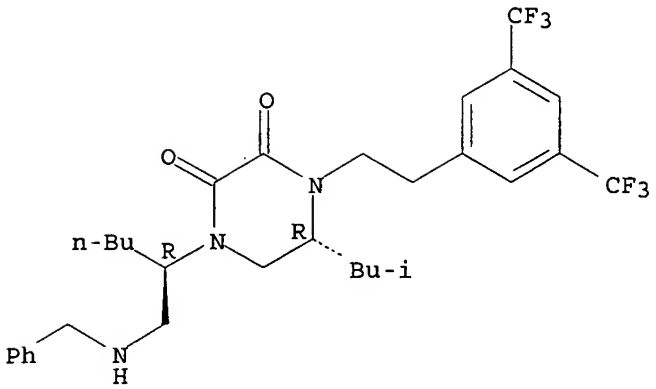
RN 537053-17-1 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-4-[2-[4-(2-methylpropyl)phenyl]propyl]-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



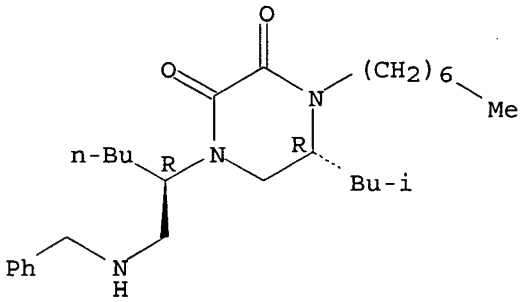
RN 537053-18-2 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



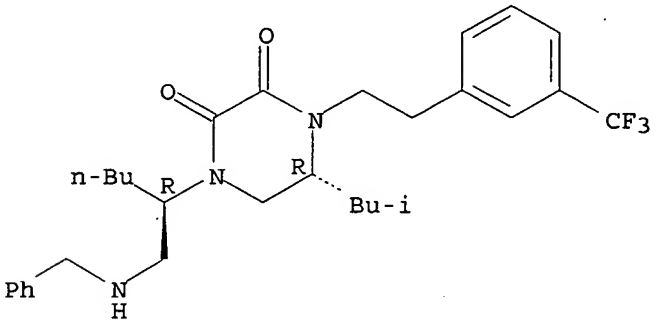
RN 537053-19-3 HCAPLUS
CN 2,3-Piperazinedione, 4-heptyl-5-(2-methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-20-6 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

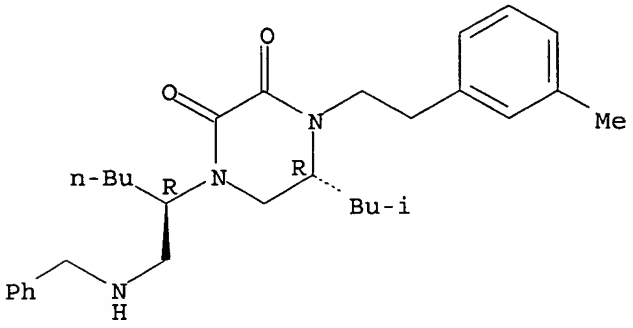
Absolute stereochemistry.



RN 537053-21-7 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-

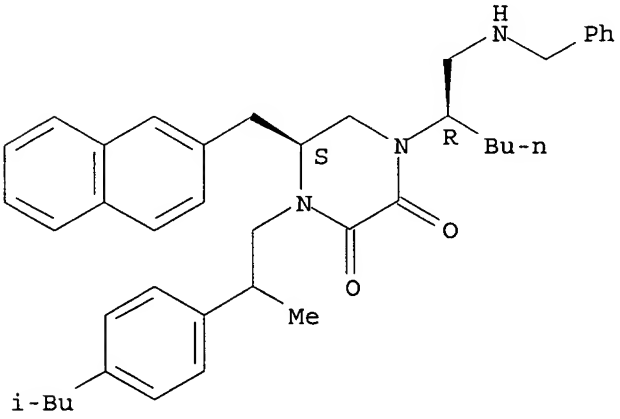
methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



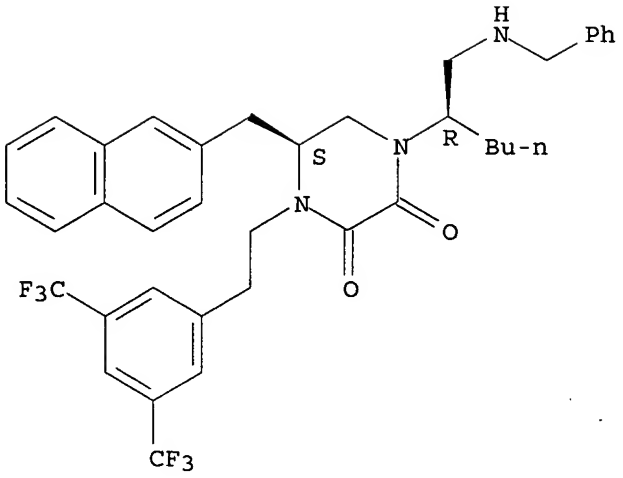
RN 537053-22-8 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[4-(2-methylpropyl)phenyl]propyl]-5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



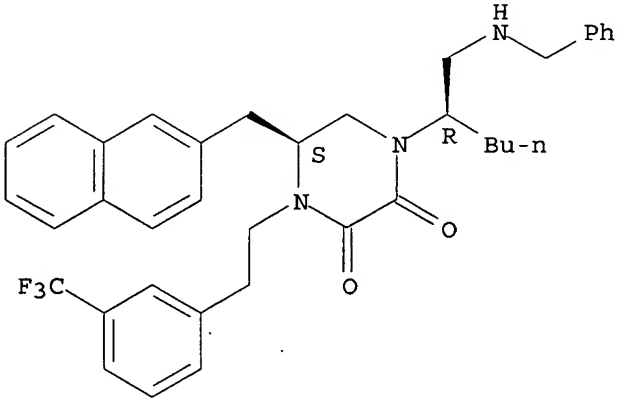
RN 537053-23-9 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



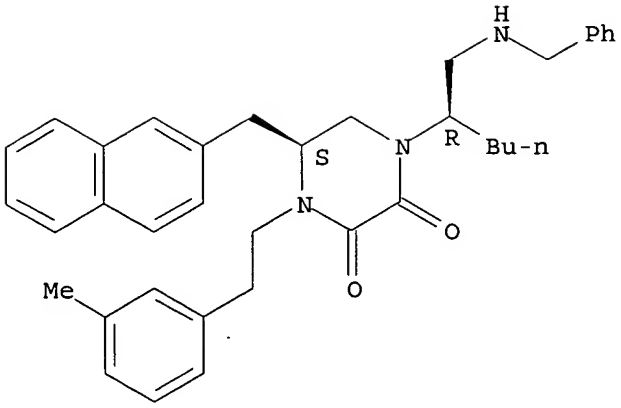
RN 537053-24-0 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



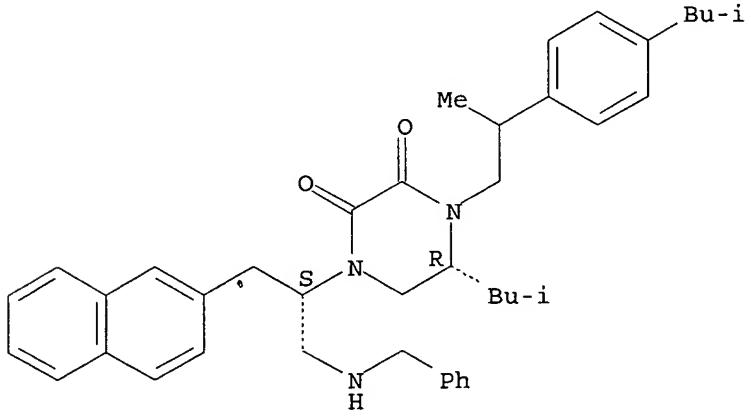
RN 537053-25-1 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



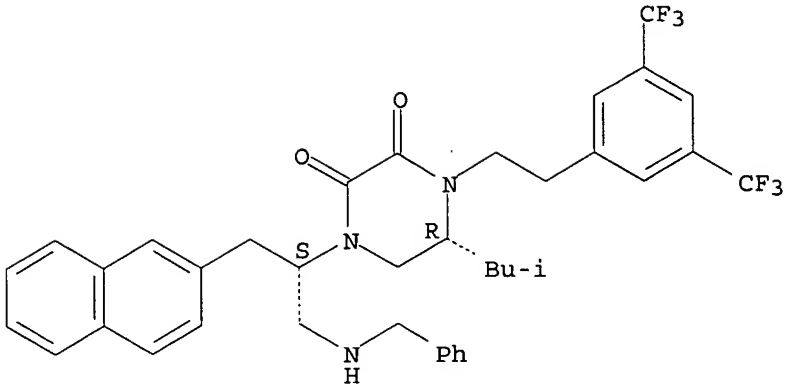
RN 537053-26-2 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-4-[2-[4-(2-methylpropyl)phenyl]propyl]-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



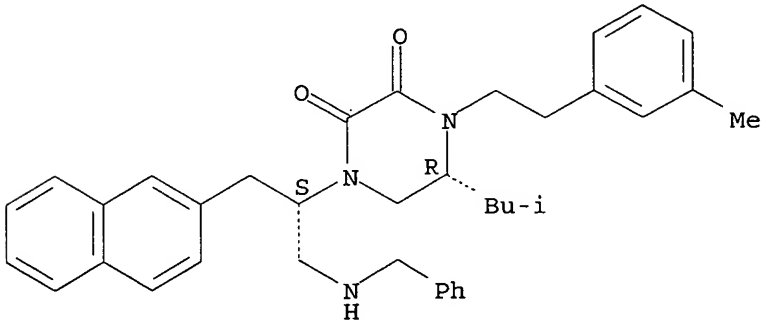
RN 537053-27-3 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-methylpropyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



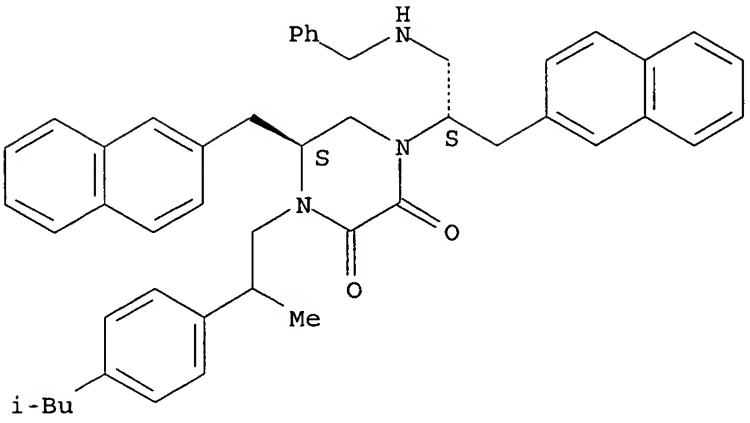
RN 537053-28-4 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-methylpropyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-29-5 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[4-(2-methylpropyl)phenyl]propyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-30-8 HCAPLUS
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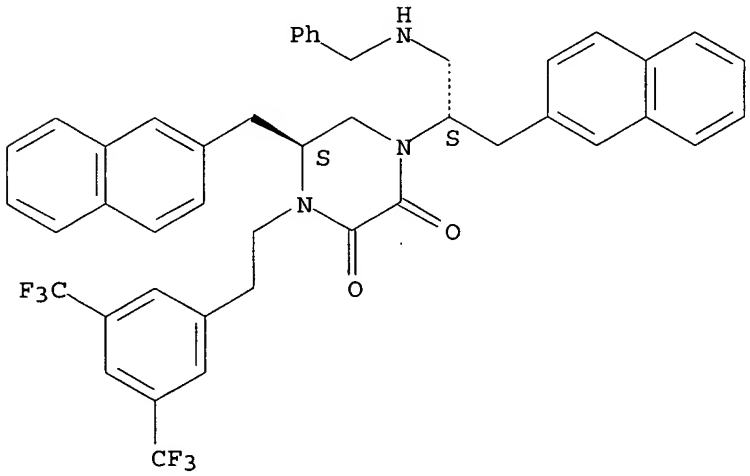
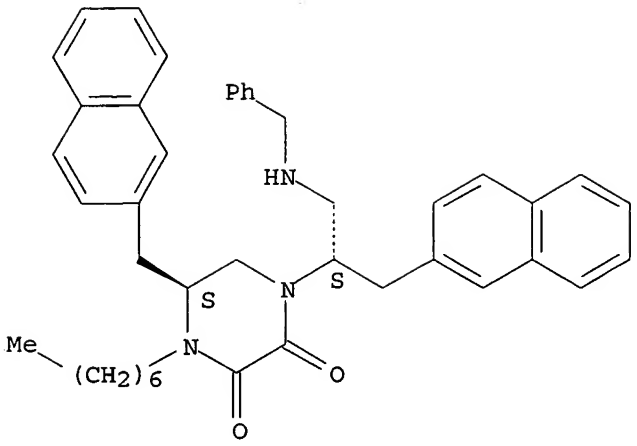
Absolute stereochemistry.



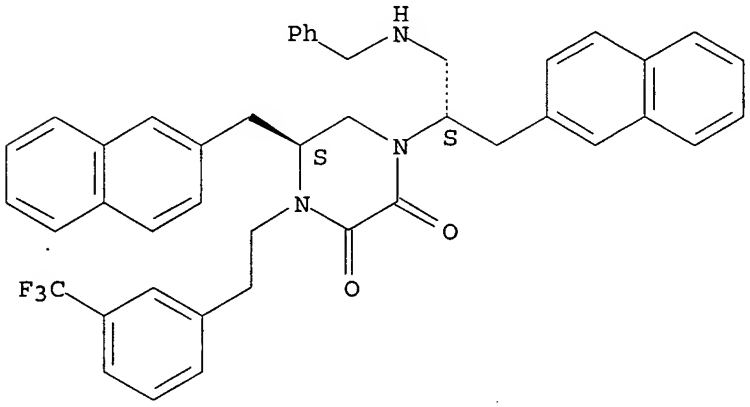
RN 537053-31-9 HCAPLUS
CN 2,3-Piperazinedione, 4-heptyl-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



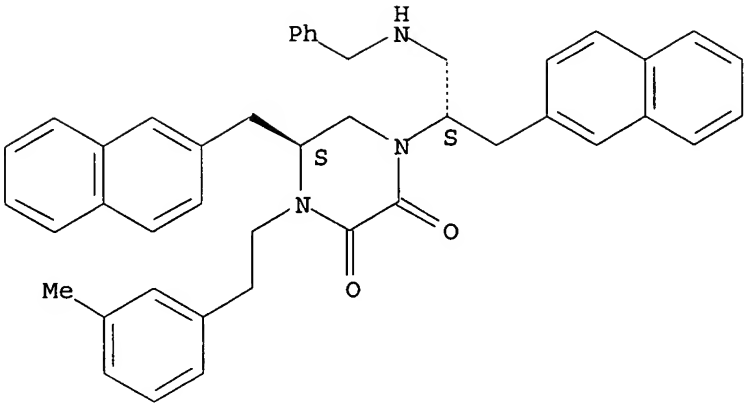
RN 537053-32-0 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-33-1 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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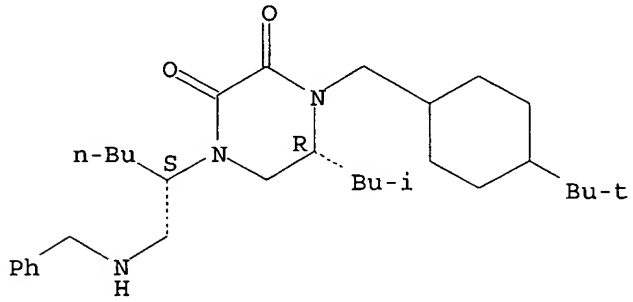
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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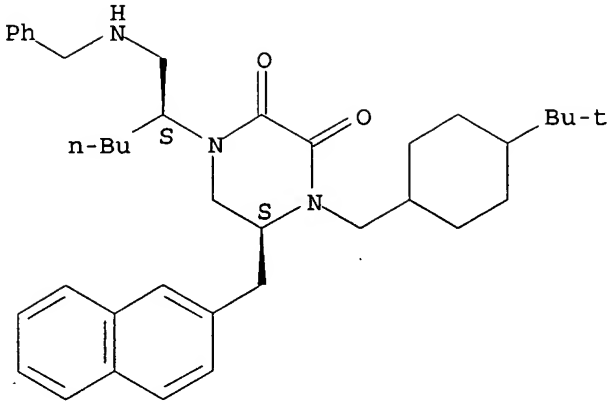
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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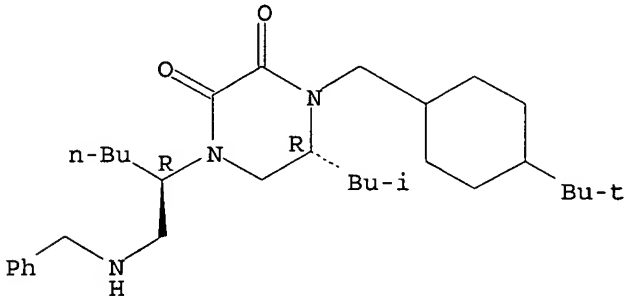
Absolute stereochemistry.



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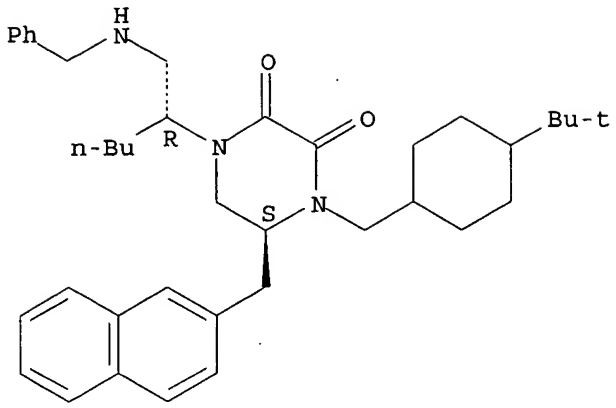
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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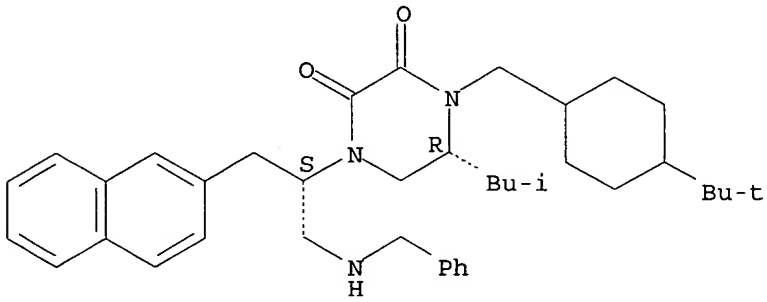
Absolute stereochemistry.



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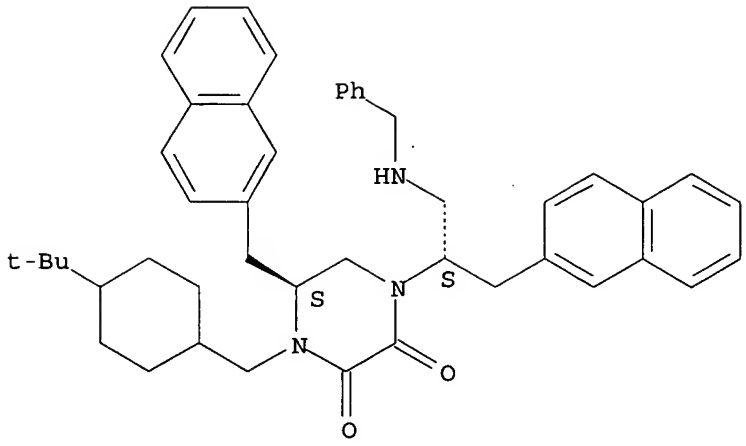
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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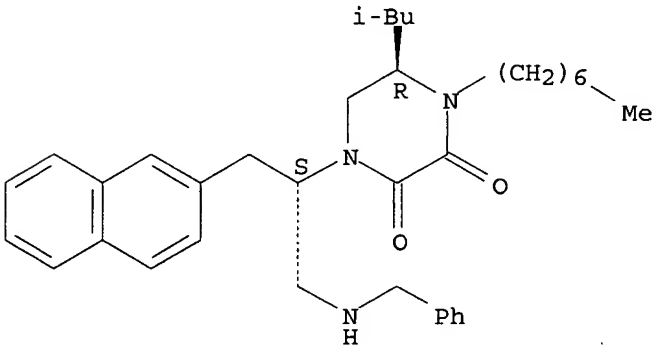
CN 2,3-Piperazinedione, 4-heptyl-5-(2-methylpropyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C12N009-99
ICS A61K038-52
INCL 514012000; 435325000; 435184000
CC 1-6 (Pharmacology)
Section cross-reference(s): 7
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(peptidyl and nonpeptidyl compds. for derepression of IAP-inhibited caspase and therapeutic and drug screening uses)

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(peptidyl and nonpeptidyl compds. for derepression of IAP-inhibited caspase and therapeutic and drug screening uses)

L10 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:434582 HCAPLUS
DOCUMENT NUMBER: 139:30774
TITLE: Methods and compositions using peptidyl and nonpeptidyl compounds for derepression of IAP-inhibited caspase, therapeutic use, and methods for identification of agents
INVENTOR(S): Reed, John C.; Houghten, Richard A.; Nefzi, Adel; Ostresh, John M.; Pinilla, Clemencia; Welsh, Kate
PATENT ASSIGNEE(S): The Burnham Institute, USA; Torrey Pines Institute for Molecular Studies
SOURCE: PCT Int. Appl., 182 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003045974	A2	20030605	WO 2002-US37577	2002 1121
WO 2003045974	A3	20040219		
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CA 2467892	AA	20030605	CA 2002-2467892	

				2002 1121
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CN 1615148	A	20050511	CN 2002-827412	2002 1121
PRIORITY APPLN. INFO.:			US 2001-331957P P	2001 1121
			WO 2002-US37577 W	2002 1121

AB The invention provides isolated agents having a core peptidyl or nonpeptidyl (e.g. urea derivative, diketopiperazine derivative) structure, wherein the agent derepresses an IAP-inhibited caspase. The invention also provides a method of derepressing an IAP-inhibited caspase. The method consists of contacting an IAP-inhibited caspase with an effective amount of an agent to derepress an IAP-inhibited caspase. The methods of the invention can be used for promoting apoptosis in a cell and for reducing the severity of a pathol. (e.g. cancer) characterized by reduced levels of apoptosis. Methods for identifying agents that derepress an IAP-inhibited caspase are also provided.

IT **537051-58-4 537051-59-5 537053-07-9**
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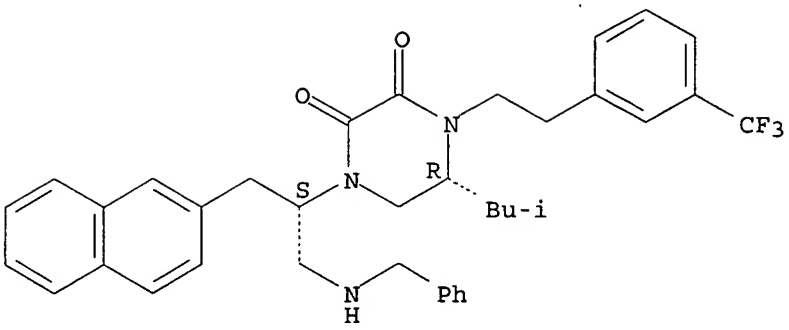
(peptidyl and nonpeptidyl compds. for derepression of IAP-inhibited caspase, therapeutic use, and methods for identification of agents)

RN 537051-58-4 HCAPLUS

CN 2,3-Piperazinedione, 5-(2-methylpropyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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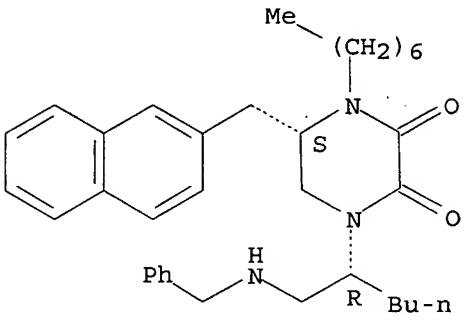
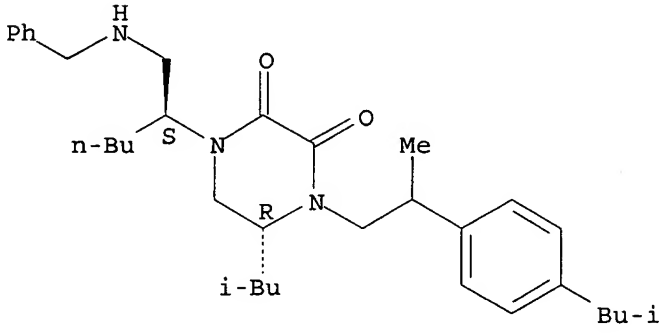
CN 2,3-Piperazinedione, 4-heptyl-5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-07-9 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-4-[2-[4-(2-methylpropyl)phenyl]propyl]-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

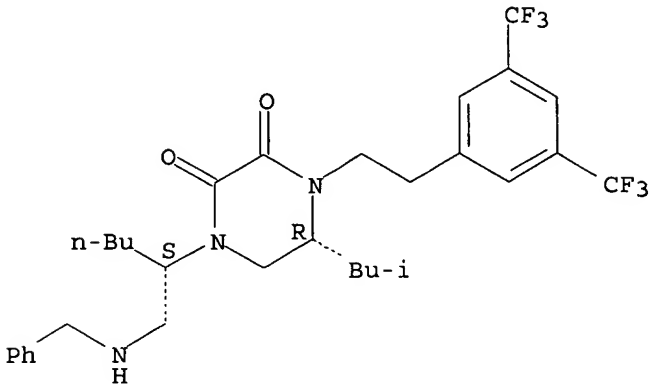
Absolute stereochemistry.



RN 537053-08-0 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-,

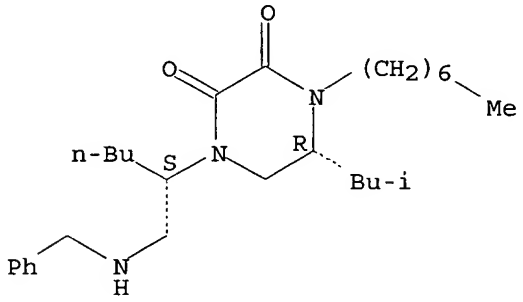
(5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



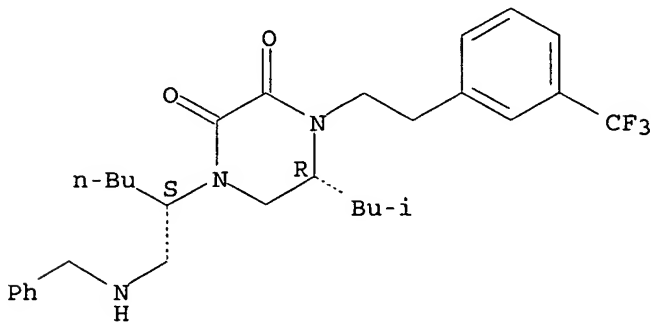
RN 537053-09-1 HCAPLUS
CN 2,3-Piperazinedione, 4-heptyl-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



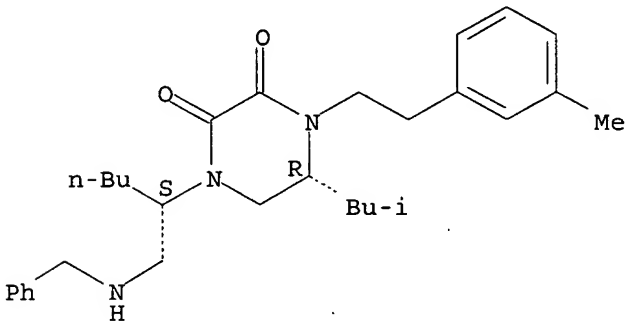
RN 537053-10-4 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



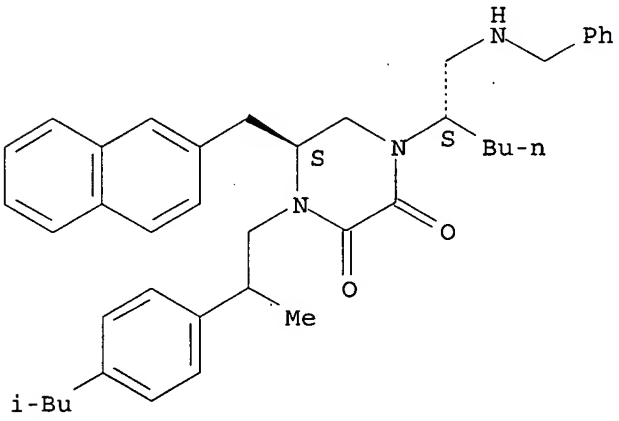
RN 537053-11-5 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



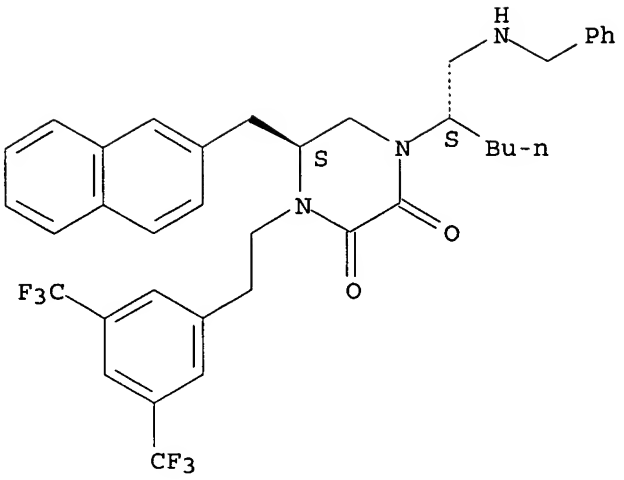
RN 537053-12-6 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[4-(2-methylpropyl)phenyl]propyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



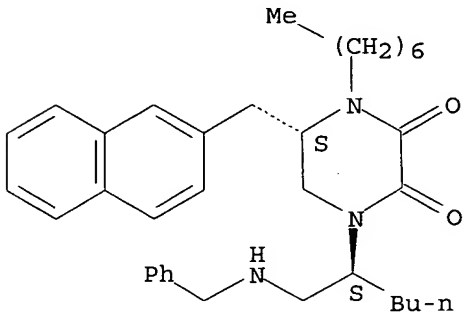
RN 537053-13-7 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



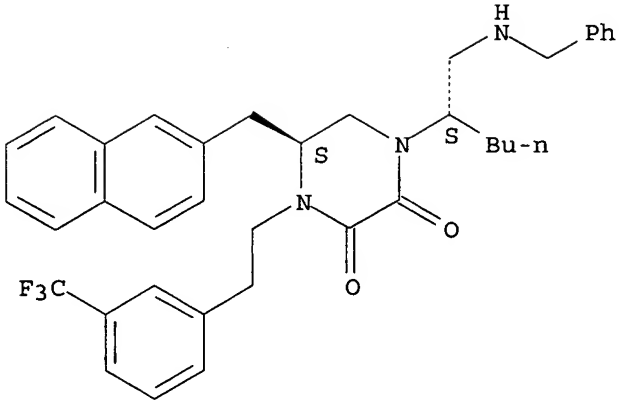
RN 537053-14-8 HCAPLUS
CN 2,3-Piperazinedione, 4-heptyl-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



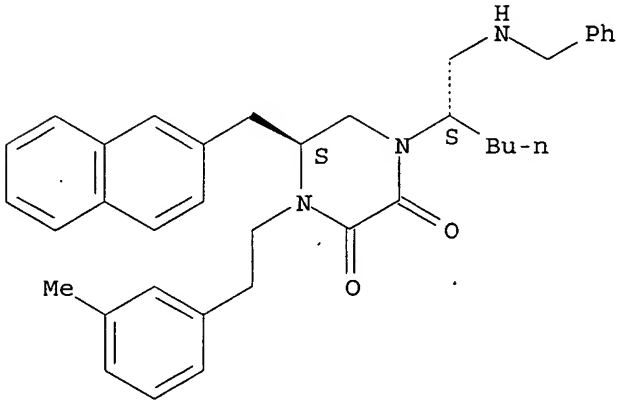
RN 537053-15-9 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



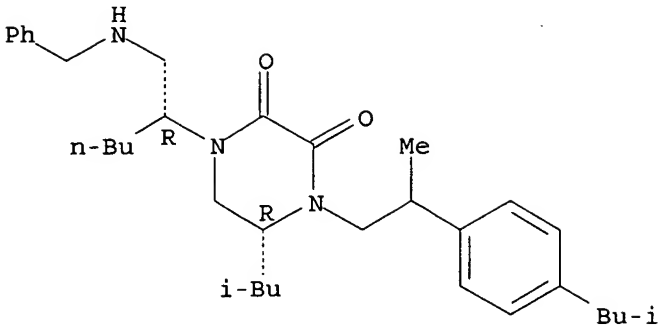
RN 537053-16-0 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-17-1 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-4-[2-[4-(2-methylpropyl)phenyl]propyl]-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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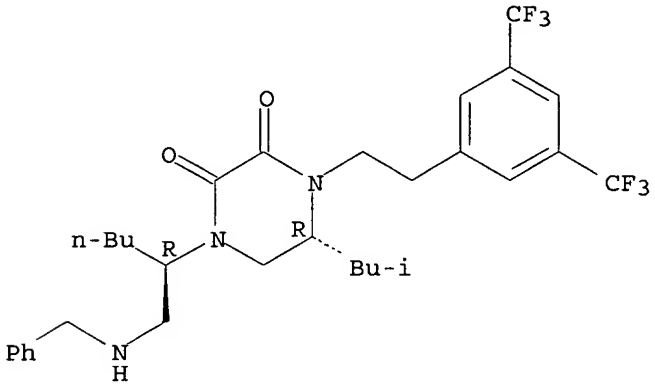
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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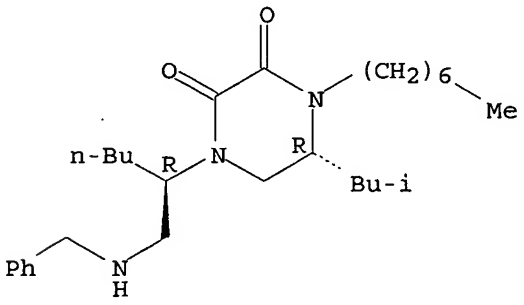
CN 2,3-Piperazinedione, 4-heptyl-5-(2-methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

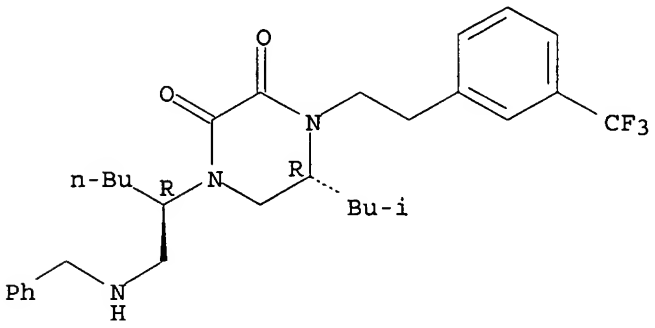
Absolute stereochemistry.



RN 537053-20-6 HCAPLUS
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-1-[(1R)-1-

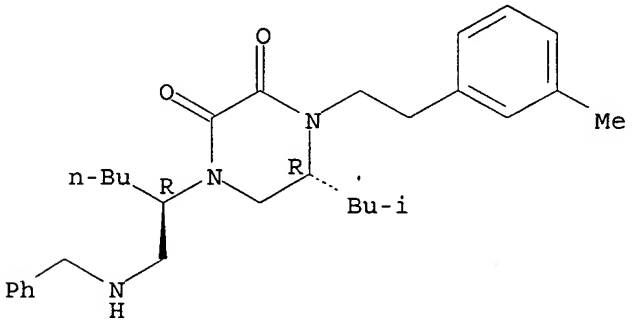
[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



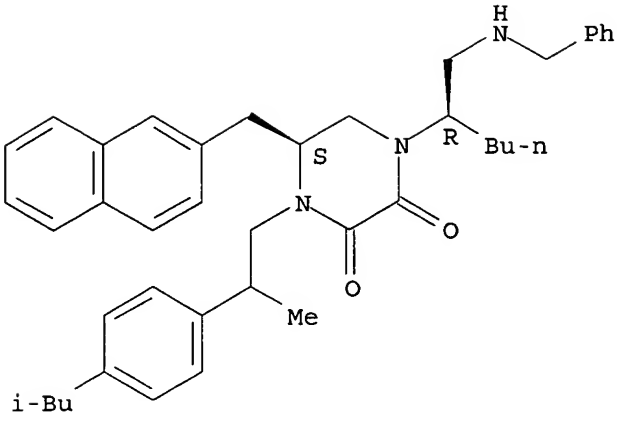
RN 537053-21-7 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



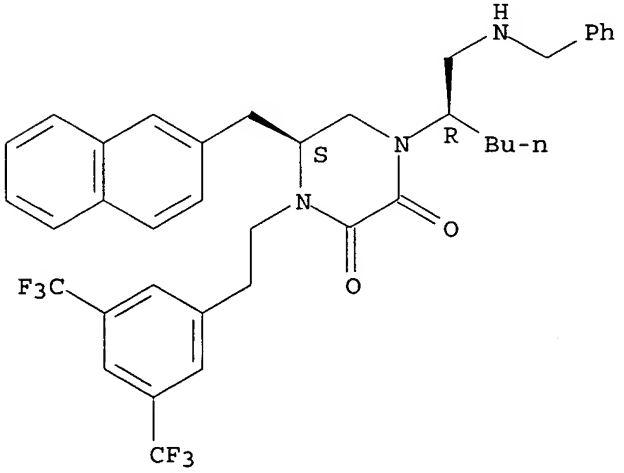
RN 537053-22-8 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[4-(2-methylpropyl)phenyl]propyl]-5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-23-9 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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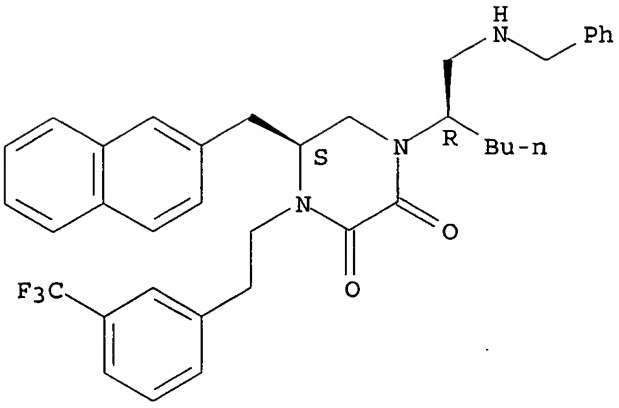
CN 2,3-Piperazinedione, 5-(2-naphthalenylmethyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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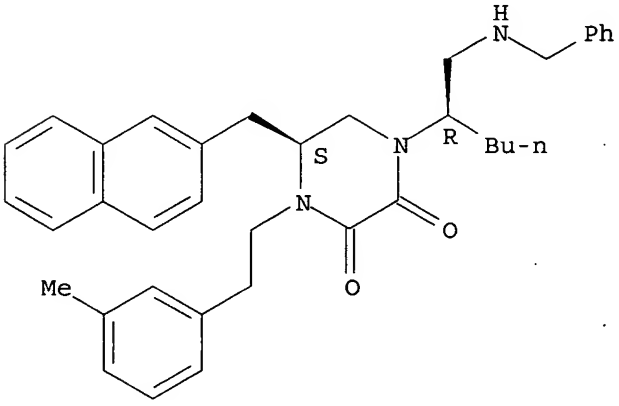
Absolute stereochemistry.



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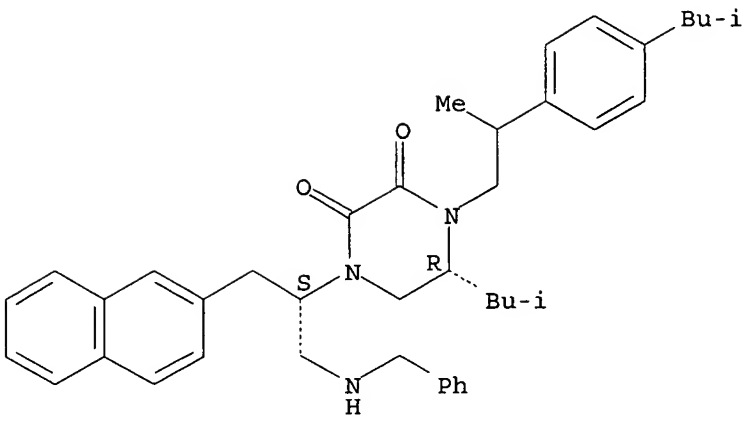
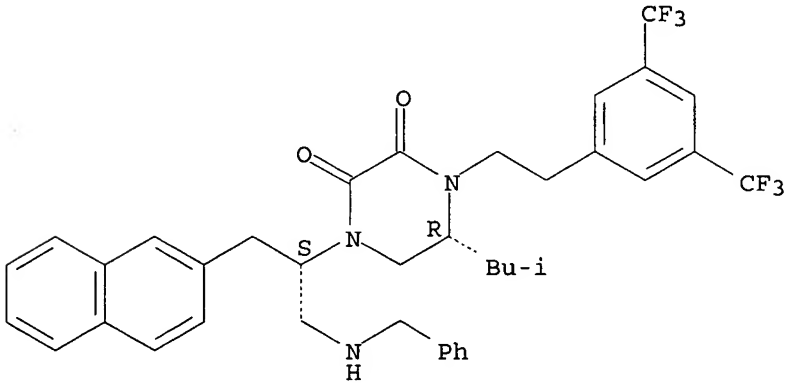
CN 2,3-Piperazinedione, 5-(2-methylpropyl)-4-[2-[4-(2-methylpropyl)phenyl]propyl]-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-27-3 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-methylpropyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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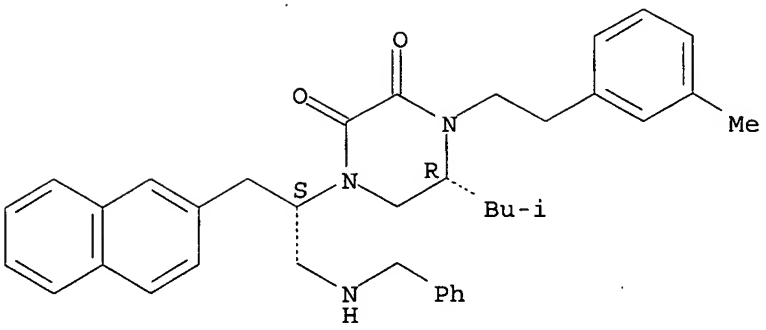
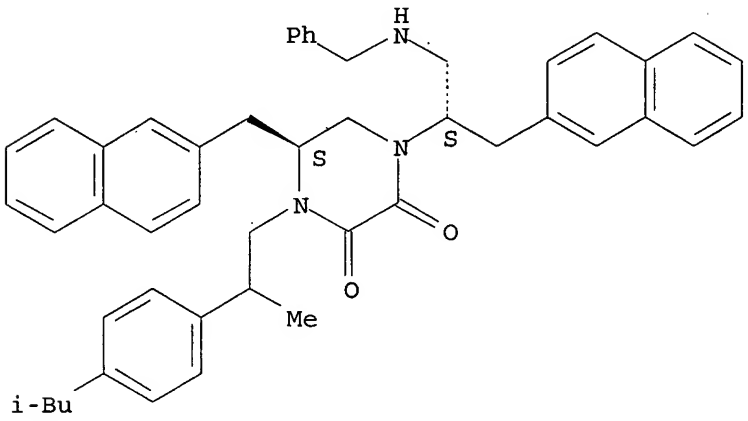
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-methylpropyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



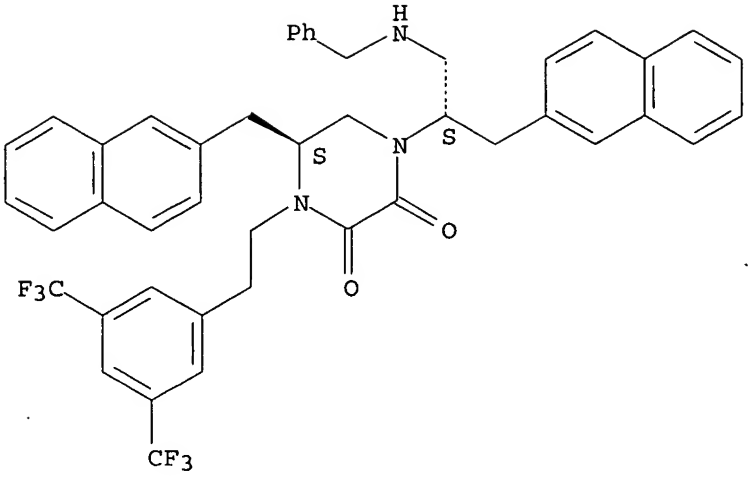
RN 537053-29-5 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[4-(2-methylpropyl)phenyl]propyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



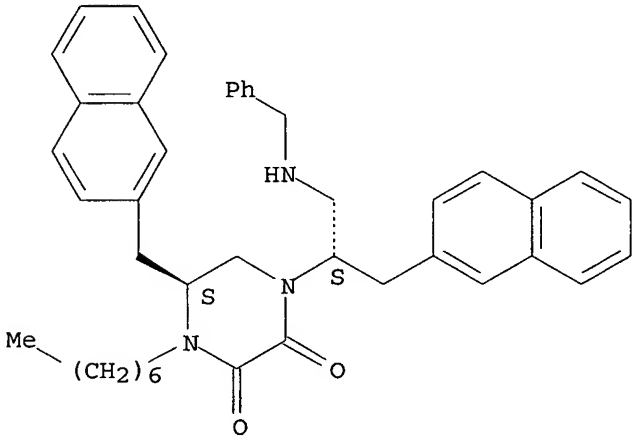
RN 537053-30-8 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537053-31-9 HCAPLUS
CN 2,3-Piperazinedione, 4-heptyl-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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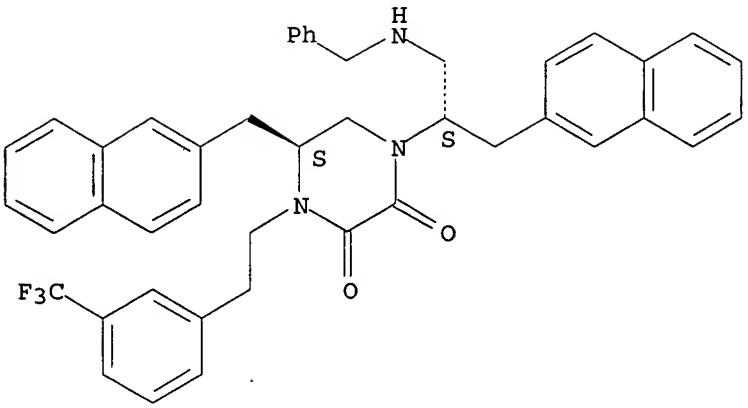
CN 2,3-Piperazinedione, 5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-4-[2-[3-(trifluoromethyl)phenyl]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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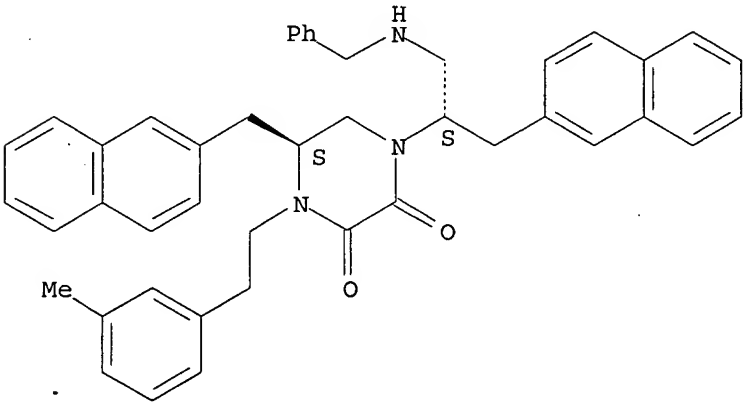
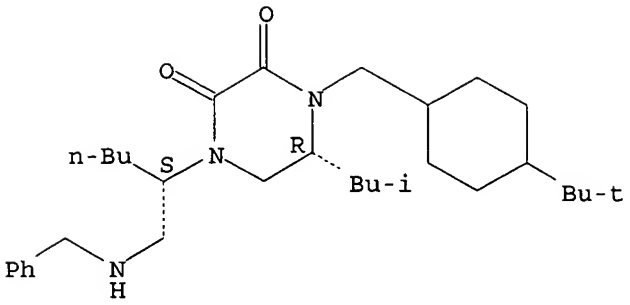
CN 2,3-Piperazinedione, 4-[2-(3-methylphenyl)ethyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-(2-naphthalenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



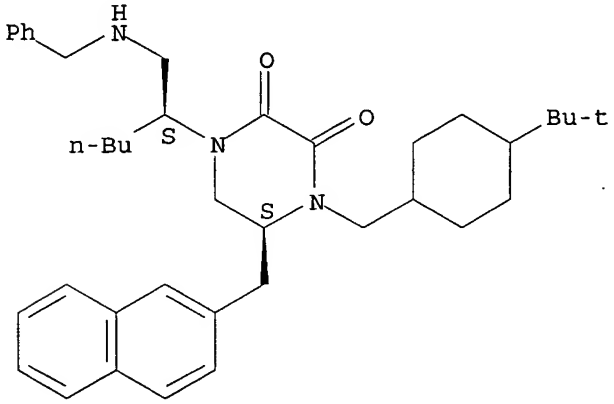
RN 540529-39-3 HCAPLUS
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-(2-methylpropyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



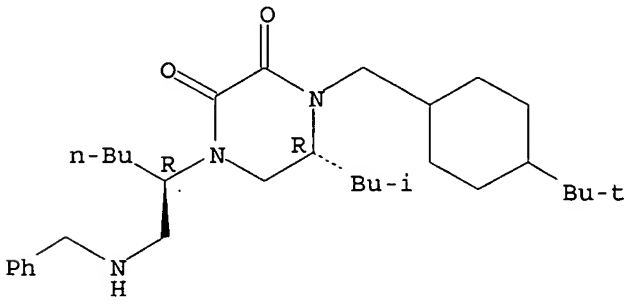
RN 540529-41-7 HCAPLUS
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-(2-naphthalenylmethyl)-1-[(1S)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 540529-43-9 HCAPLUS
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-(2-methylpropyl)-1-[(1R)-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 540529-46-2 HCAPLUS
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-

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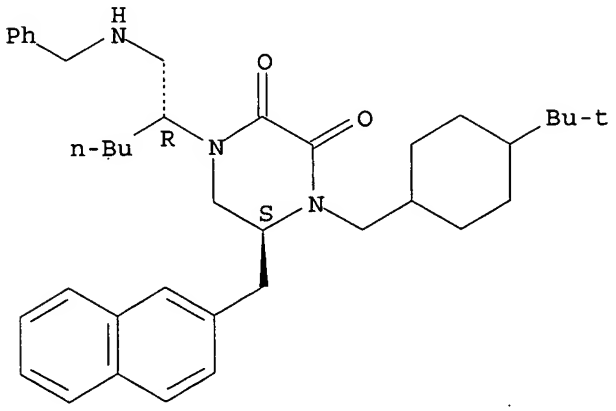
yl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 540529-48-4 HCAPLUS
CN 2,3-Piperazinedione, 4-[[4-(1,1-dimethylethyl)cyclohexyl]methyl]-5-
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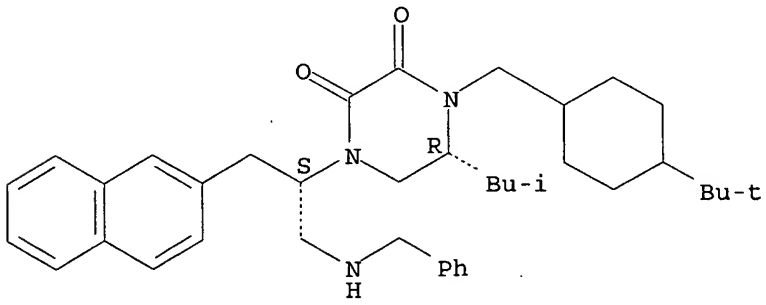
Absolute stereochemistry.



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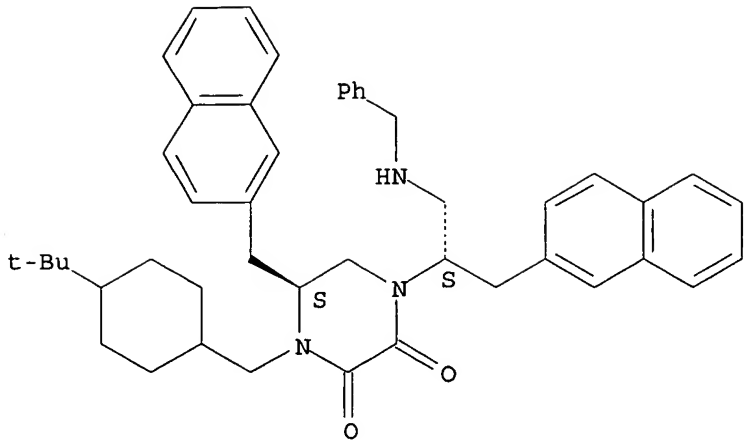
Absolute stereochemistry.



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(peptidyl and nonpeptidyl compds. for derepression of IAP-inhibited caspase, therapeutic use, and methods for identification of agents)

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L10 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:655115 HCAPLUS
DOCUMENT NUMBER: 137:185839
TITLE: Preparation of diketodiazacyclic compounds, diazacyclic compounds and combinatorial libraries
INVENTOR(S): Nefzi, Adel; Ostresh, John M.; Houghten, Richard A.
PATENT ASSIGNEE(S): Torrey Pines Institute for Molecular Studies, USA
SOURCE: U.S., 43 pp., Cont.-in-part of U.S. 5,786,448. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6441172	B1	20020827	US 1999-310662	1999 0512
US 5786448	A	19980728	US 1996-745793	1996

All 3 of 1PPs Same

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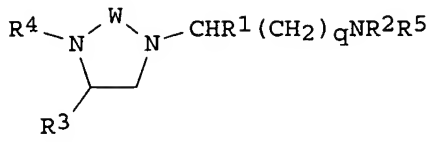

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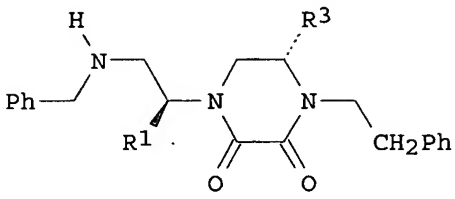


II

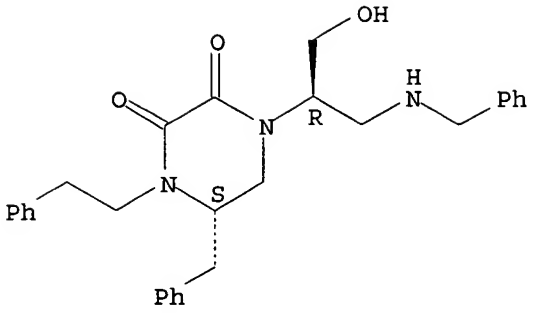
AB 1,4-Diazacyclic compds. I [q = 1-7; W is an (un)saturated chain of 2-4 carbon atoms which may be substituted by one or two oxo groups and other substituents and two of the remaining carbon atoms of the chain form an (un)saturated mono- or bicyclic ring containing 5- to 8-members in each ring and zero to three heteroatoms in each ring that are independently oxygen, nitrogen or sulfur; R1, R3 = H, (un)substituted alkyl, phenylalkyl, Ph, cycloalkyl; R2 = alkyl, alkenyl, (un)substituted benzyl or naphthyl; R4 = H, (un)substituted alkyl or phenylalkenyl, alkenyl, substituted cycloalkyl, phenylalkyl; R5 = H, acyl, aroyl, alkyl- or arylaminocarbonyl or -thiocarbonyl] and libraries of these compds. were prepared Thus, diketopiperazines II [R1 = monosubstituted benzyl, s-Bu, CH2OH, Me, (CH2)4NMeCH2Ph; R3 = PhCH2, CHMe2] were prepared by forming resin-bound N-acylated dipeptides, reduction of the amide groups, cyclization, and cleavage from the resin. Preparation of combinatorial libraries of N-benzyl- or N-methyl-1,4,5-trisubstituted-2,3-diketopiperazines and N-methyl-5,7-diketo-1,4-diazacycloheptanes are also described. The N-benzyl-1,4,5-trisubstituted-2,3-diketopiperazine library compds. were screened for orphanin binding and binding inhibition of the rat brain mu receptor.

IT **287495-20-9P 287495-21-0P 287495-22-1P**
287495-24-3P 287495-25-4P 287495-39-0P
308133-16-6P 308133-18-8P 308133-20-2P
308133-24-6P
(solid-phase synthesis of diketodiazacyclic compds., diazacyclic compds. and combinatorial libraries)

RN 287495-20-9 HCAPLUS

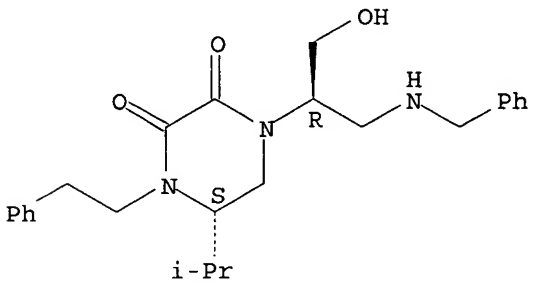
CN 2,3-Piperazinedione, 1-[(1R)-1-(hydroxymethyl)-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



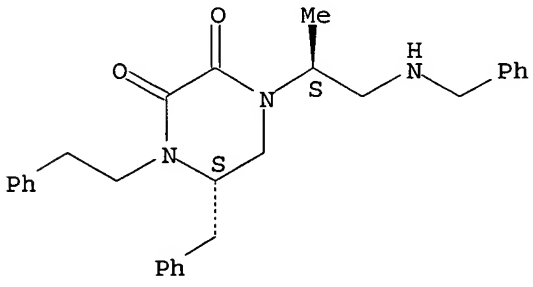
RN 287495-21-0 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1R)-1-(hydroxymethyl)-2-[(phenylmethyl)amino]ethyl]-5-(1-methylethyl)-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



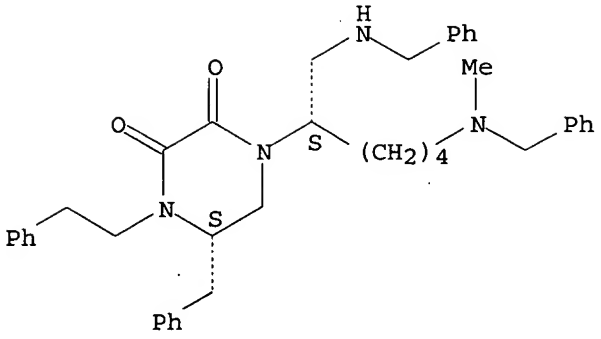
RN 287495-22-1 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-1-methyl-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



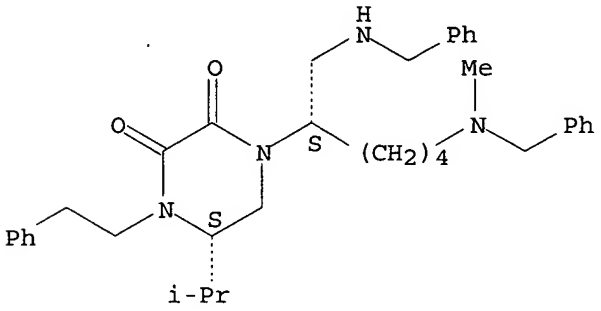
RN 287495-24-3 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



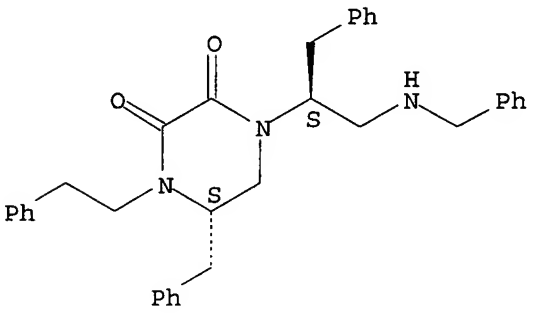
RN 287495-25-4 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



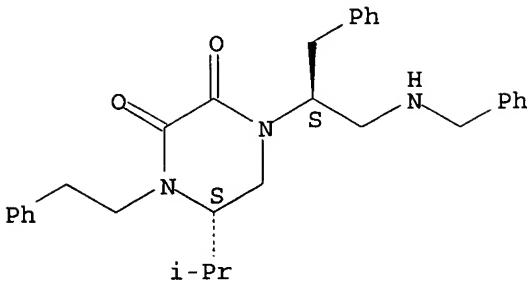
RN 287495-39-0 HCAPLUS
CN 2,3-Piperazinedione, 4-(2-phenylethyl)-5-(phenylmethyl)-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



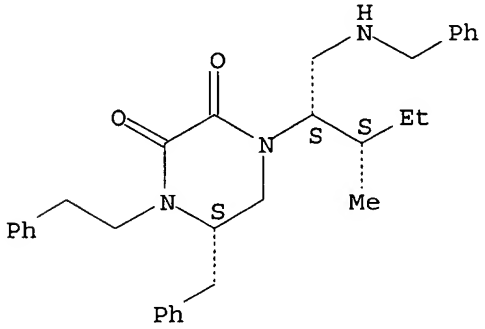
RN 308133-16-6 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-4-(2-phenylethyl)-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



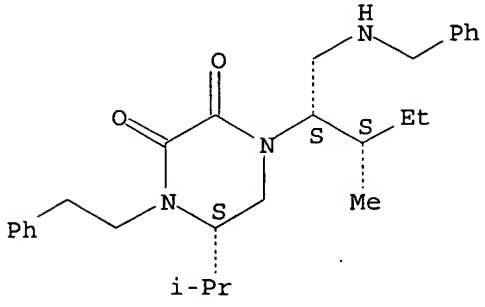
RN 308133-18-8 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S,2S)-2-methyl-1-[[(phenylmethyl)amino]methyl]butyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



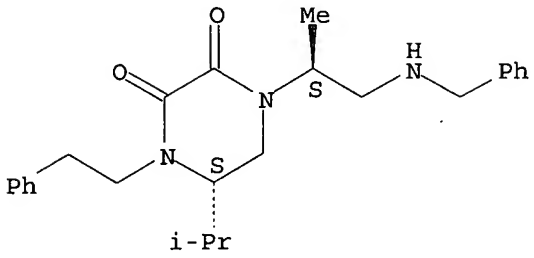
RN 308133-20-2 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-1-[(1S,2S)-2-methyl-1-[[(phenylmethyl)amino]methyl]butyl]-4-(2-phenylethyl)-, (5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 308133-24-6 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-1-[(1S)-1-methyl-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



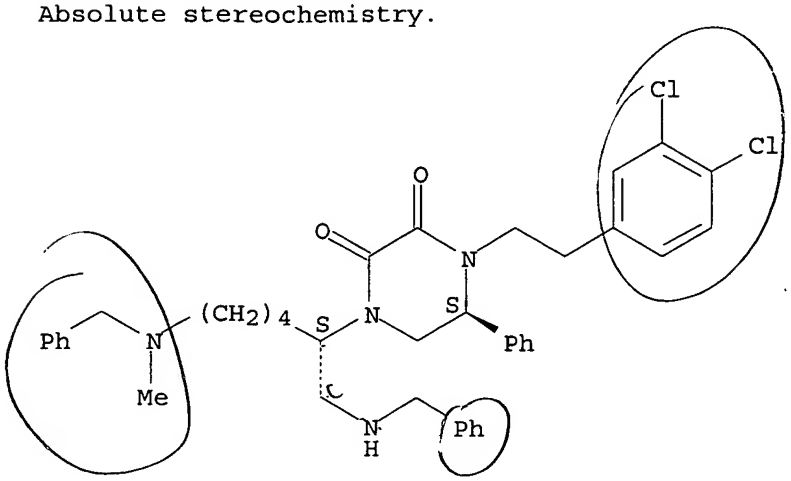
IC ICM C07D241-04
INCL 544383000
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 2, 28
IT 71754-91-1P 256663-69-1P 256663-70-4P 256663-71-5P
256663-72-6P 256663-73-7P 256663-77-1P 256663-78-2P
256663-79-3P 287495-08-3P 287495-09-4P 287495-11-8P
287495-12-9P 287495-13-0P 287495-15-2P **287495-20-9P**
287495-21-0P 287495-22-1P 287495-24-3P
287495-25-4P 287495-39-0P 308132-92-5P
308132-97-0P 308133-02-0P 308133-07-5P 308133-12-2P
308133-16-6P 308133-18-8P 308133-20-2P
308133-24-6P
(solid-phase synthesis of diketodiazacyclic compds., diazacyclic compds. and combinatorial libraries)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:46830 HCAPLUS
DOCUMENT NUMBER: 137:185430
TITLE: Solid phase synthesis of acyclic and heterocyclic combinatorial libraries from resin-bound triamines
AUTHOR(S): Nefzi, Adel; Giulianotti, Marc A.; Ong, Nhi A.; Ostresh, John M.; Dooley, Colette T.; Blondelle, Sylvie E.; Houghten, Richard A.
CORPORATE SOURCE: Torrey Pines Institute for Molecular Studies, San Diego, CA, 92121, USA
SOURCE: Innovation and Perspectives in Solid Phase Synthesis & Combinatorial Libraries: Peptides, Proteins and Nucleic Acids--Small Molecule Organic Chemistry Diversity, Collected Papers, International Symposium, 6th, York, United Kingdom, Aug. 31-Sept. 4, 1999 (2001), Meeting Date 1999, 119-122. Editor(s): Epton, Roger. Mayflower Scientific Ltd.: Kingswinford, UK.
CODEN: 69CEGV; ISBN: 0-9515735-3-5
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A symposium report. Acyclic and heterocyclic synthetic combinatorial libraries (SCLs) were prepared from peptide SCLs using the "libraries from libraries" approach. A bicyclic guanidine library was screened in a radioreceptor assay selective for the κ opiate receptor. A number of compds. showed binding affinities < 200 nM.

3 of APP's
NO Dup Comp.

IT **449778-38-5P**
(solid phase synthesis of acyclic and heterocyclic combinatorial libraries from resin-bound triamines)
RN 449778-38-5 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3,4-dichlorophenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-phenyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 25, 34
IT **449778-38-5P** 449778-39-6P
(solid phase synthesis of acyclic and heterocyclic combinatorial libraries from resin-bound triamines)
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:824229 HCAPLUS
DOCUMENT NUMBER: 134:5160
TITLE: Preparation of diketodiazacyclic compounds, diazacyclic compounds and combinatorial libraries
INVENTOR(S): Nefzi, Adel; Ostresh, John M.; Houghten, Richard A.
PATENT ASSIGNEE(S): Torrey Pines Institute for Molecular Studies, USA
SOURCE: PCT Int. Appl., 165 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000069830	A1	20001123	WO 2000-US10841	2000 0421

W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CR, CU, CZ, DM, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR,

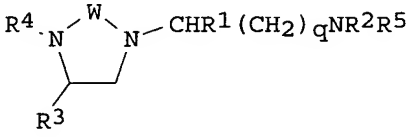
LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SD, SG, SI, SK, TR, TT, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6441172	B1	20020827	US 1999-310662	1999 0512
CA 2373590	AA	20001123	CA 2000-2373590	2000 0421
EP 1181279	A1	20020227	EP 2000-926259	2000 0421
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AU 774270	B2	20040624	AU 2000-44818	2000 0421

PRIORITY APPLN. INFO.:	US 1999-310662	A 1999 0512
	US 1996-745793	A2 1996 1107
	WO 2000-US10841	W 2000 0421

OTHER SOURCE(S): MARPAT 134:5160

GI



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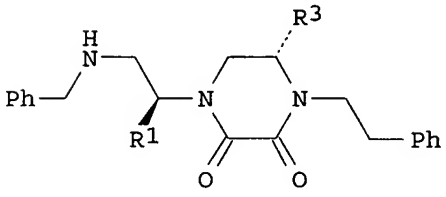


II

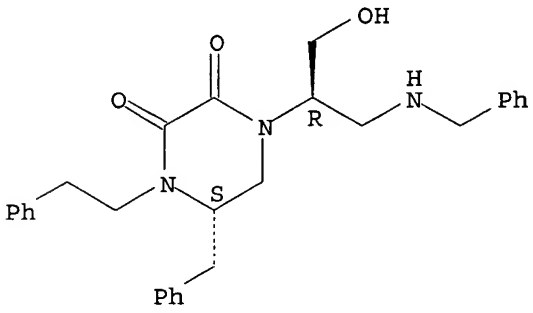
AB 1,4-Diazacyclic compds. I [q = 1-7; W is an (un)saturated chain of 2-4 carbon atoms which may be substituted by one or two oxo groups and other substituents and two of the remaining carbon atoms of the chain form an (un)saturated mono- or bicyclic ring containing 5- to 8-members in each ring and zero to three heteroatoms in each ring that are independently oxygen, nitrogen or sulfur; R1, R3 = H,

(un)substituted alkyl, phenylalkyl, Ph, cycloalkyl; R2 = alkyl, alkenyl, (un)substituted benzyl or naphthyl; R4 = H, (un)substituted alkyl or phenylalkenyl, alkenyl, substituted cycloalkyl, phenylalkyl; R5 = H, acyl, aroyl, alkyl- or arylaminocarbonyl or -thiocarbonyl] and libraries of these compds. were prepared Thus, diketopiperazines II [R1 = monosubstituted benzyl, s-Bu, CH2OH, Me, (CH2)4NMeCH2Ph; R3 = PhCH2, CHMe2] were prepared by forming resin-bound N-acylated dipeptides, reduction of the amide groups, cyclization, and cleavage from the resin.

IT **287495-20-9P 287495-21-0P 287495-22-1P**
287495-24-3P 287495-25-4P 287495-39-0P
308133-16-6P 308133-18-8P 308133-20-2P
308133-24-6P
(solid-phase synthesis of diketodiazacyclic compds., diazacyclic compds. and combinatorial libraries)

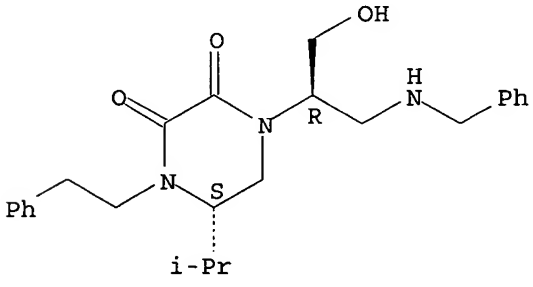
RN 287495-20-9 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1R)-1-(hydroxymethyl)-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



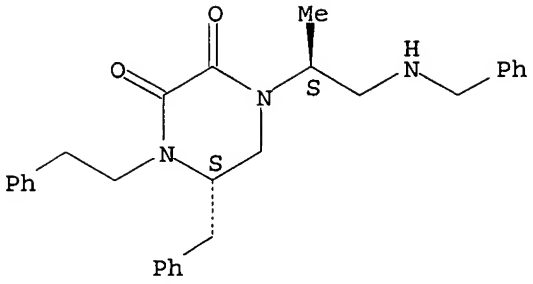
RN 287495-21-0 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1R)-1-(hydroxymethyl)-2-[(phenylmethyl)amino]ethyl]-5-(1-methylethyl)-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



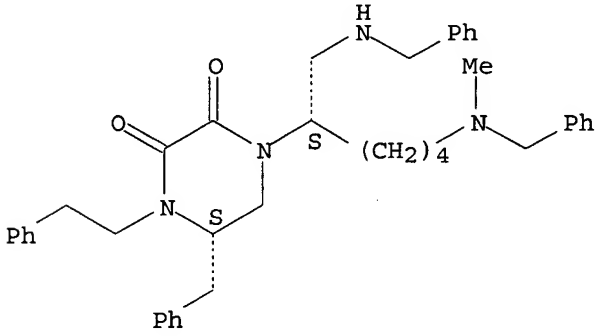
RN 287495-22-1 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-1-methyl-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



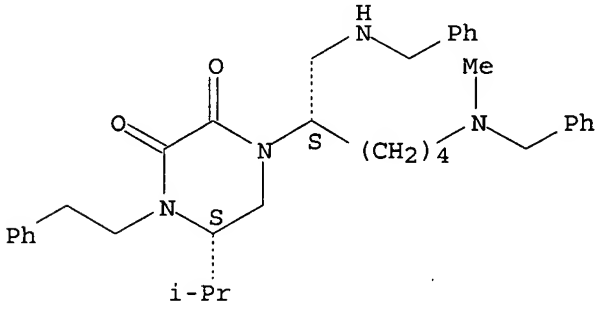
RN 287495-24-3 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



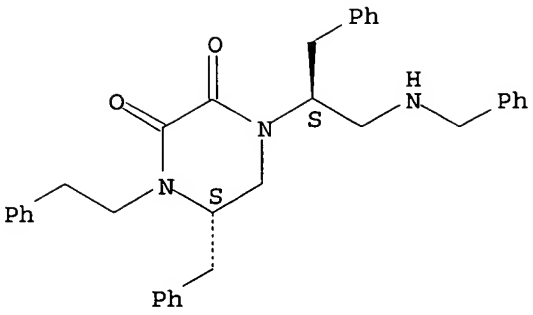
RN 287495-25-4 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



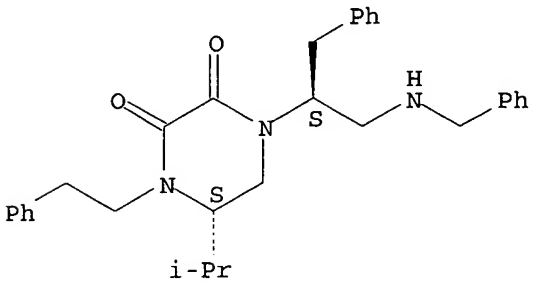
RN 287495-39-0 HCAPLUS
CN 2,3-Piperazinedione, 4-(2-phenylethyl)-5-(phenylmethyl)-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



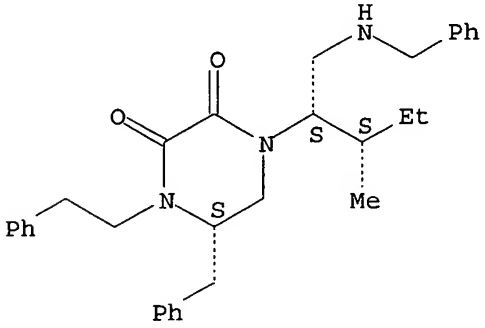
RN 308133-16-6 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-4-(2-phenylethyl)-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



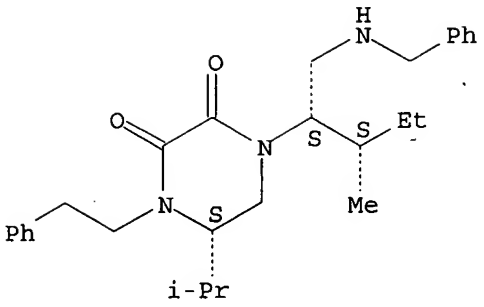
RN 308133-18-8 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S,2S)-2-methyl-1-[[(phenylmethyl)amino]methyl]butyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



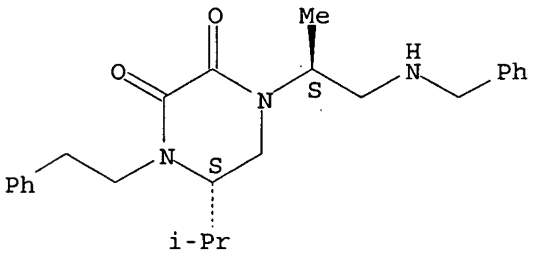
RN 308133-20-2 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-1-[(1S,2S)-2-methyl-1-[[(phenylmethyl)amino]methyl]butyl]-4-(2-phenylethyl)-, (5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 308133-24-6 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-1-[(1S)-1-methyl-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07D223-00
ICS C07D225-00; C07D241-04; C07D245-00; C07D267-02; G01N033-536; G01N033-543
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 28
IT 71754-91-1P 256663-69-1P 256663-70-4P 256663-71-5P
256663-72-6P 256663-73-7P 256663-77-1P 256663-78-2P
256663-79-3P 287495-08-3P 287495-09-4P 287495-11-8P
287495-12-9P 287495-13-0P 287495-15-2P **287495-20-9P**
287495-21-0P 287495-22-1P 287495-24-3P
287495-25-4P 287495-39-0P 308132-92-5P
308132-97-0P 308133-02-0P 308133-07-5P 308133-12-2P
308133-16-6P 308133-18-8P 308133-20-2P
308133-24-6P
(solid-phase synthesis of diketodiazacyclic compds., diazacyclic compds. and combinatorial libraries)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:373661 HCAPLUS
DOCUMENT NUMBER: 133:150895
TITLE: Solid-phase synthesis of substituted 2,3-diketopiperazines from reduced polyamides
AUTHOR(S): Nefzi, Adel; Giulianotti, Marc A.; Houghten, Richard A.
CORPORATE SOURCE: Torrey Pines Institute for Molecular Studies,

#14650
2 of Appl's
102(b)

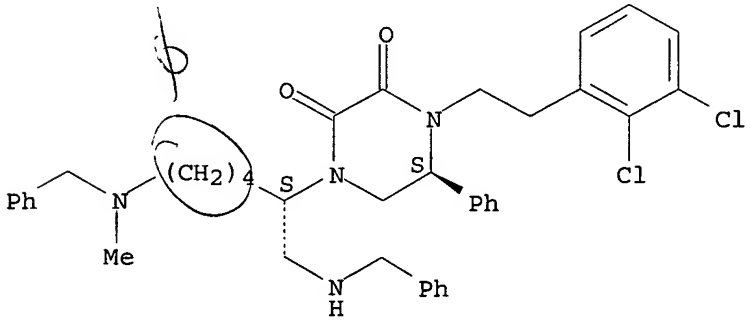
San Diego, CA, 92121, USA
SOURCE: Tetrahedron (2000), 56(21), 3319-3326
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:150895

AB An efficient method for the solid phase synthesis of 1,6-disubstituted 2,3-diketopiperazine and 1,4,5-trisubstituted 2,3-diketopiperazine derivs. is described. The reduction of resin-bound acylated amino acids or resin-bound acylated dipeptides, followed by treatment with oxalyldiimidazole, affords the corresponding diketopiperazines in good yield and high purity. This is an example of a broader approach to the solid phase synthesis of individual heterocyclic compds. using peptides directly or indirectly as starting materials.

IT **287495-16-3P 287495-17-4P 287495-18-5P**
287495-19-6P 287495-20-9P 287495-21-0P
287495-22-1P 287495-23-2P 287495-24-3P
287495-25-4P 287495-26-5P 287495-27-6P
287495-28-7P 287495-30-1P 287495-31-2P
287495-32-3P 287495-33-4P 287495-34-5P
287495-35-6P 287495-36-7P 287495-37-8P
287495-38-9P 287495-39-0P
(solid-phase synthesis of substituted 2,3-diketopiperazines from reduced polyamides)

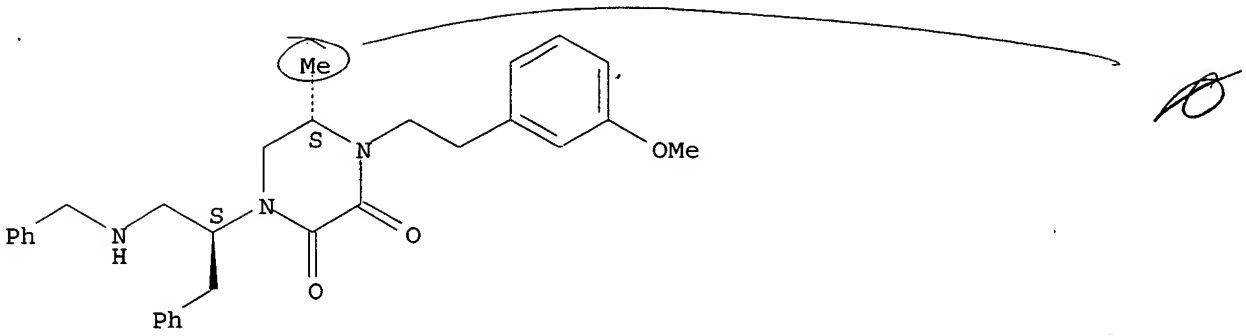
RN 287495-16-3 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(2,3-dichlorophenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-phenyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



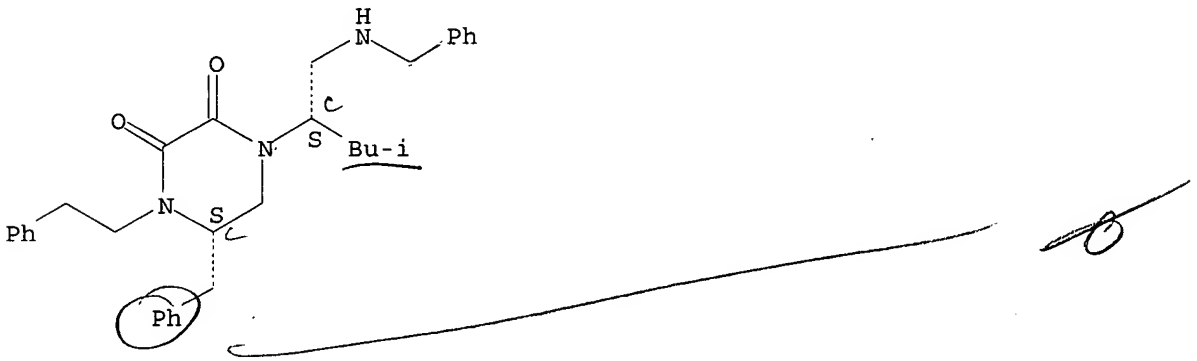
RN 287495-17-4 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(3-methoxyphenyl)ethyl]-5-methyl-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



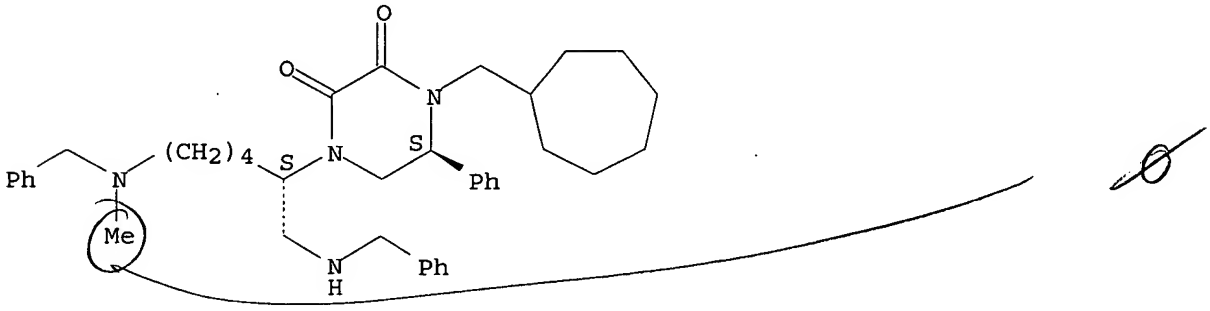
RN 287495-18-5 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-3-methyl-1-[[(phenylmethyl)amino]methyl]butyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



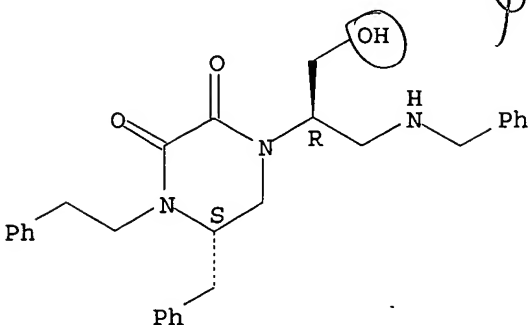
RN 287495-19-6 HCAPLUS
CN 2,3-Piperazinedione, 4-(cycloheptylmethyl)-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-phenyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



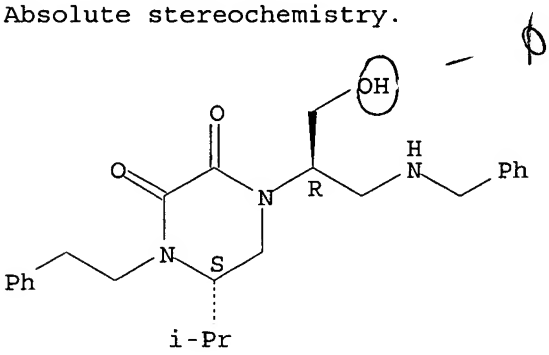
RN 287495-20-9 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1R)-1-(hydroxymethyl)-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



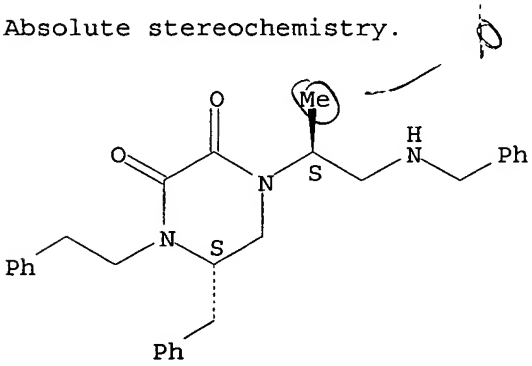
RN 287495-21-0 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1R)-1-(hydroxymethyl)-2-[(phenylmethyl)amino]ethyl]-5-(1-methylethyl)-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



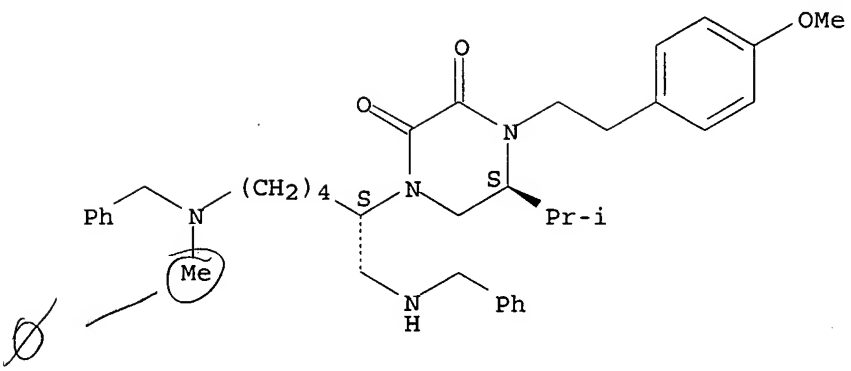
RN 287495-22-1 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-1-methyl-2-[(phenylmethyl)amino]ethyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



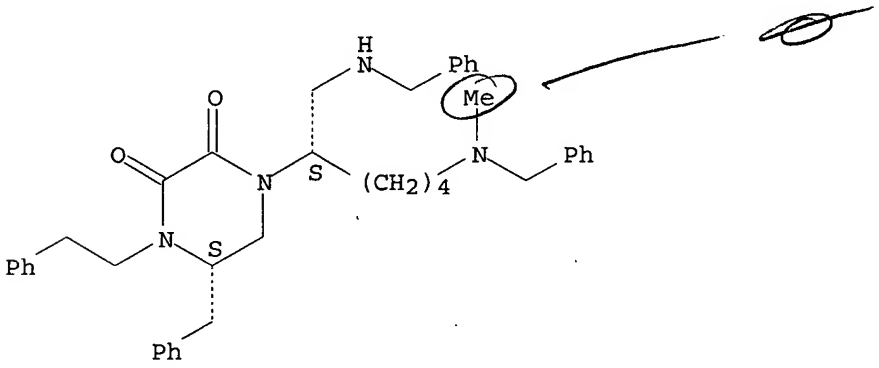
RN 287495-23-2 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-methoxyphenyl)ethyl]-5-(1-methylethyl)-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



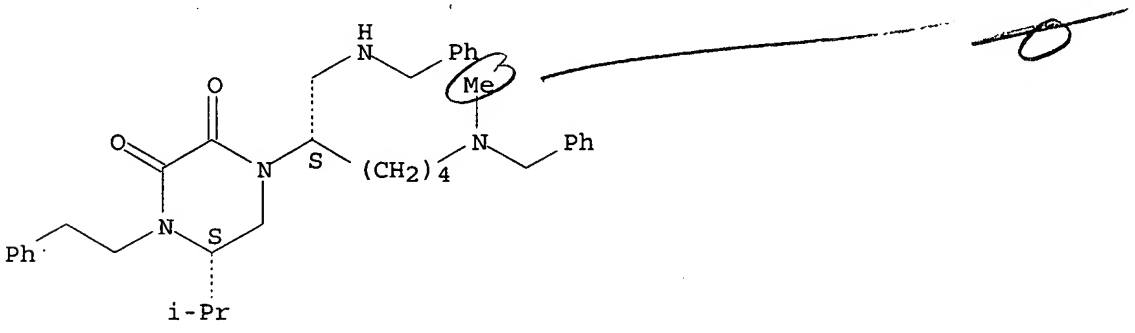
RN 287495-24-3 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-4-(2-phenylethyl)-5-(phenylmethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



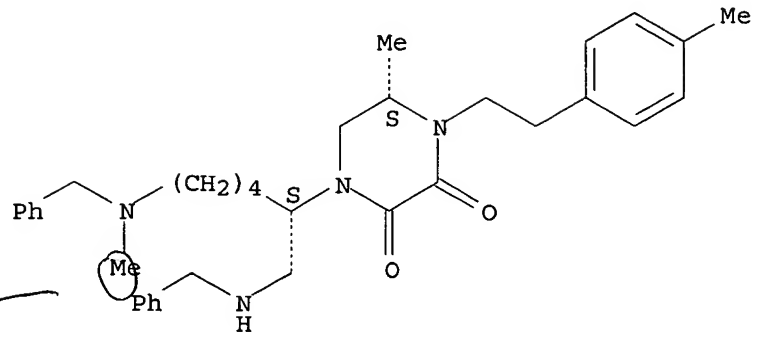
RN 287495-25-4 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-4-(2-phenylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



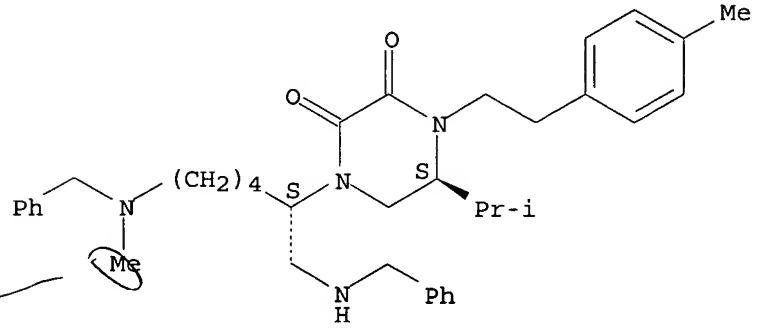
RN 287495-26-5 HCAPLUS
CN 2,3-Piperazinedione, 5-methyl-4-[2-(4-methylphenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



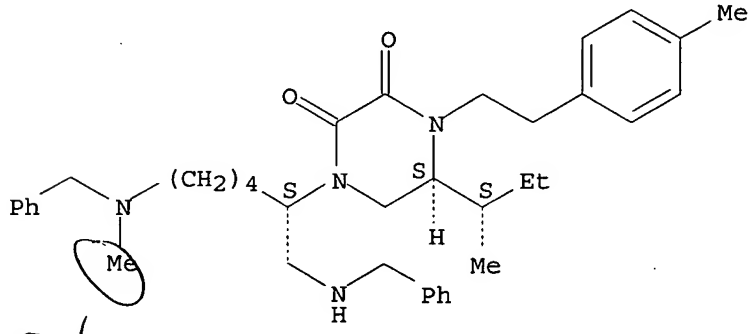
RN 287495-27-6 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-4-[2-(4-methylphenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



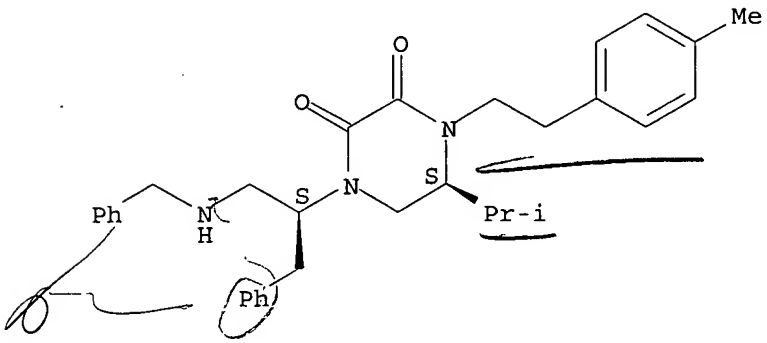
RN 287495-28-7 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-methylphenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-[(1S)-1-methylpropyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



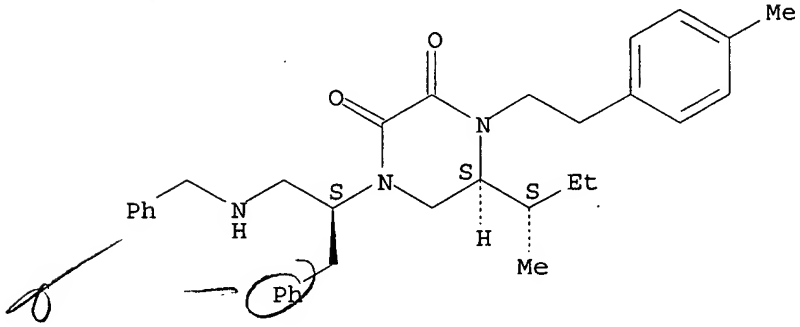
RN 287495-30-1 HCAPLUS
CN 2,3-Piperazinedione, 5-(1-methylethyl)-4-[2-(4-methylphenyl)ethyl]-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



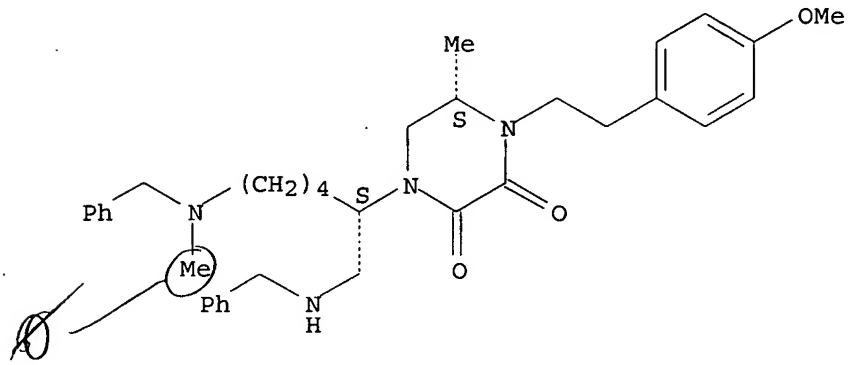
RN 287495-31-2 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-methylphenyl)ethyl]-5-[(1S)-1-methylpropyl]-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



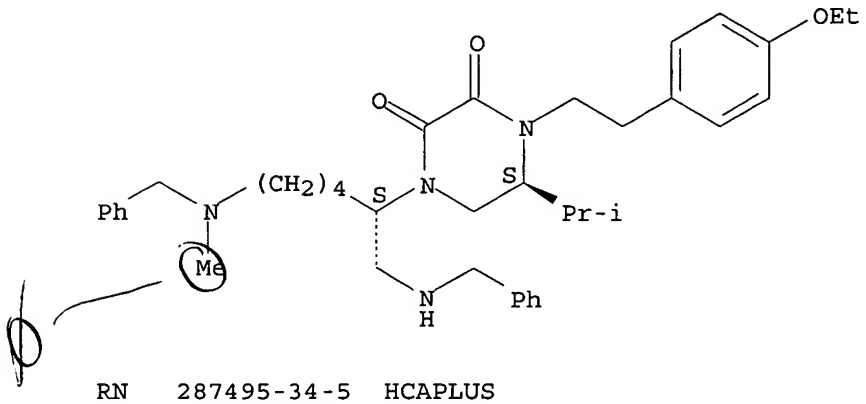
RN 287495-32-3 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-methoxyphenyl)ethyl]-5-methyl-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



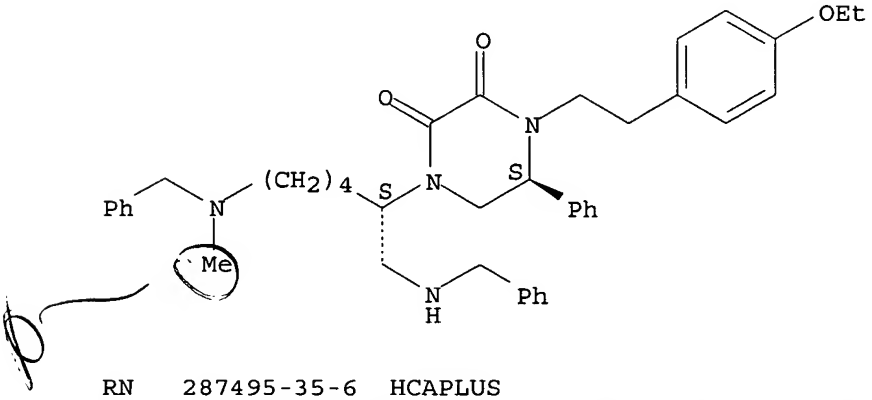
RN 287495-33-4 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-ethoxyphenyl)ethyl]-5-(1-methylethyl)-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



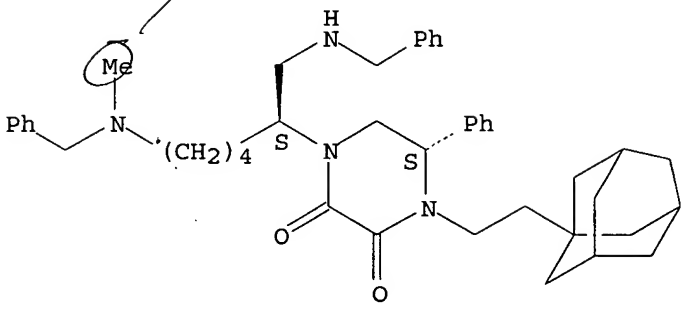
RN 287495-34-5 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-ethoxyphenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-phenyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



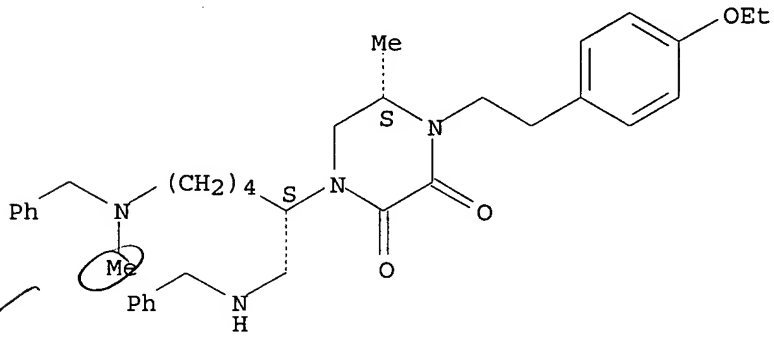
RN 287495-35-6 HCAPLUS
CN 2,3-Piperazinedione, 1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-phenyl-4-(2-tricyclo[3.3.1.13,7]dec-1-ylethyl)-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



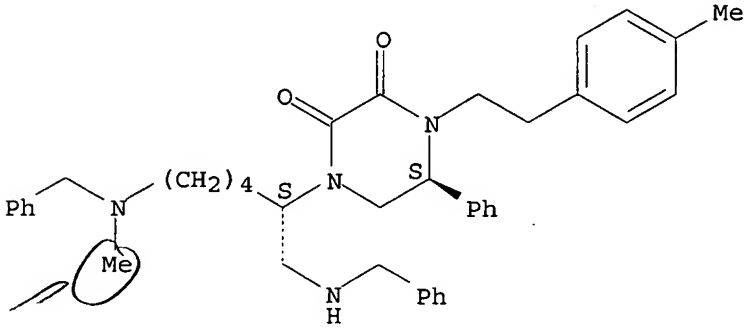
RN 287495-36-7 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-ethoxyphenyl)ethyl]-5-methyl-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



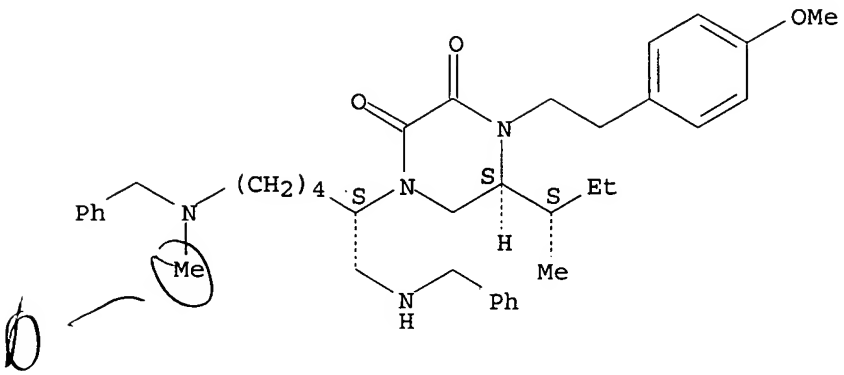
RN 287495-37-8 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-methylphenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-phenyl-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



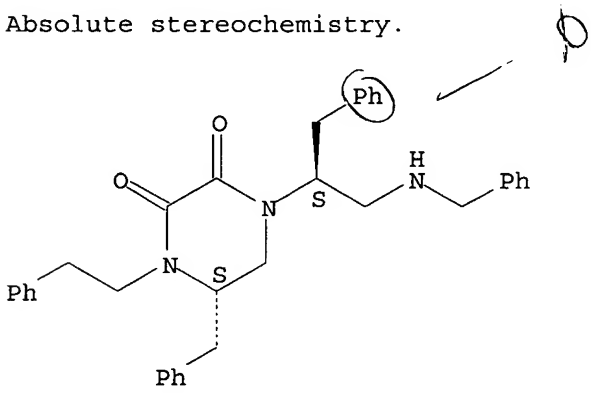
RN 287495-38-9 HCAPLUS
CN 2,3-Piperazinedione, 4-[2-(4-methoxyphenyl)ethyl]-1-[(1S)-5-[methyl(phenylmethyl)amino]-1-[[(phenylmethyl)amino]methyl]pentyl]-5-[(1S)-1-methylpropyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287495-39-0 HCAPLUS
CN 2,3-Piperazinedione, 4-(2-phenylethyl)-5-(phenylmethyl)-1-[(1S)-1-(phenylmethyl)-2-[(phenylmethyl)amino]ethyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 28
IT 71754-91-1P 256663-69-1P 256663-70-4P 256663-71-5P
256663-73-7P 256663-74-8P 256663-75-9P 256663-76-0P
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287495-36-7P 287495-37-8P 287495-38-9P
287495-39-0P
(solid-phase synthesis of substituted 2,3-diketopiperazines from reduced polyamides)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

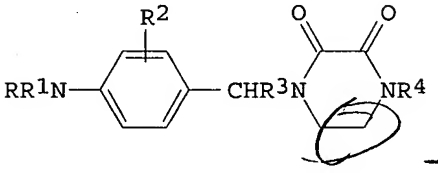
L10 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:407331 HCAPLUS

DOCUMENT NUMBER: 95:7331
TITLE: 1-(4-Aminobenzyl)-2,3-dioxopiperazine derivatives and their acid addition salts
PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan
SOURCE: Ger. Offen., 86 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3027106	A1	19810219	DE 1980-3027106	19800717
DE 3027106	C2	19881110		
JP 56018969	A2	19810223	JP 1979-93234	19790724
JP 05057272	B4	19930823		
CA 1131640	A1	19820914	CA 1980-356116	19800714
GB 2056976	A	19810325	GB 1980-23879	19800722
FR 2461705	A1	19810206	FR 1980-16275	19800723
FR 2461705	B1	19830318		

PRIORITY APPLN. INFO.: JP 1979-93234 A 19790724

OTHER SOURCE(S): MARPAT 95:7331
GI



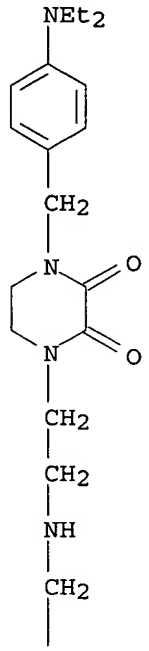
I

AB Piperazinediones I (R, R1 = H, alkyl, cycloalkyl, aralkyl, acyl, thiocarbamoyl, alkylthioimidoyl, amidino, heterocyclic; NRR1 = heterocyclic; R2 = H, amino, alkyl, alkoxy; R3 = H, alkyl; R4 = H, aliphatic, aryl, heterocyclic) were prepared Thus AcNHCH2CH2NH2 was reductively alkylated with 4-AcNHC6H4CHO to give 4-H2NC6H4CH2NHCH2CH2NH2 which was cyclized with di-Et oxalate to give I (R-R4 = H). The latter compound was treated with 2-bromopyrimidine to give I (R = 2-pyrimidinyl, R1-R4 = H) which was treated with PhCH2Cl to give I (R = 2-pyrimidinyl, R1-R3 = H, R4 = CH2Ph)(II). II had a min. inhibitory concentration against HeLa cells of 0.1 μg/mL.

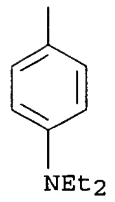
IT **77916-95-1P**

(preparation and antitumor activity of)
RN 77916-95-1 HCAPLUS
CN 2,3-Piperazinedione, 1-[[4-(diethylamino)phenyl]methyl]-4-[2-[[[4-(diethylamino)phenyl]methyl]amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●3 HCl

IC C07D241-08; A61K031-495; C07D401-00; C07D403-00
CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **77916-95-1P** 77916-97-3P 77916-98-4P 77916-99-5P
77917-01-2P 77917-02-3P 77917-05-6P 77917-10-3P
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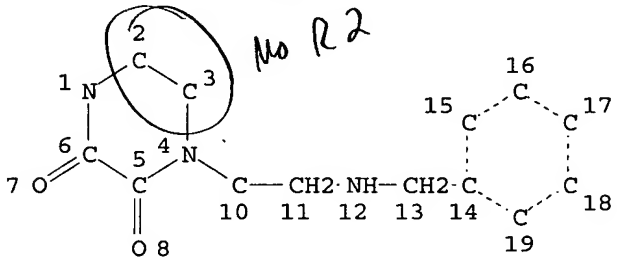
77918-04-8P 77918-05-9P 77939-48-1P
(preparation and antitumor activity of)

=> fil marpat
FILE 'MARPAT' ENTERED AT 14:27:11 ON 22 SEP 2006

=> d que l13
L7 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L9 66 SEA FILE=REGISTRY SSS FUL L7
L10 7 SEA FILE=HCAPLUS ABB=ON L9
L12 4 SEA FILE=MARPAT SSS FUL L7
L13 2 SEA FILE=MARPAT ABB=ON L12 NOT L10

=> d l13 1-2 ibib abs qhit

L13 ANSWER 1 OF 2 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 110:57692 MARPAT
TITLE: Preparation of N-benzhydrylpiperazines and analogs as vasodilators
INVENTOR(S): Hirai, Koichi; Fujimoto, Katsumi; Iwnao, Yuji; Matsui, Yoshiki
PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 76 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 283310	A1	19880921	EP 1988-302414	19880318
EP 283310	B1	19930526		

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE

US 5028610	A	19910702	US 1988-167354	19880314
JP 01063569	A2	19890309	JP 1988-64125	19880317
AT 89822	E	19930615	AT 1988-302414	19880318
CA 1326027	A1	19940111	CA 1988-561899	19880318
ES 2056913	T3	19941016	ES 1988-302414	19880318
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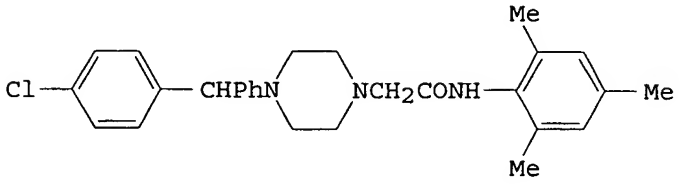
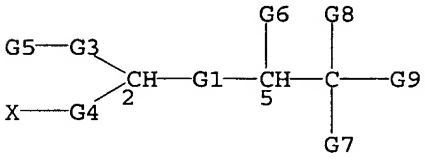


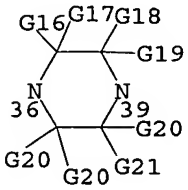
II

AB The title compds. AMB [I; A = X1C6H4CHC6H4X2; B = CHR1CR2R3NR4R5; R1 = H, alkyl; R2,R3 = H; R2R3 = O; R4,R5 = H, (un)substituted alkyl, aryl; M = 5 to 7-membered (un)substituted ring containing 2 N-atoms bearing A and B, resp., as substituents; 1 of X1,X2 = halo and the other = H, halo] were prepared 1-(4-Chlorobenzhydryl)piperazine was stirred 7.5 h at 80° with ClCH2CONHC6H2Me3-2,4,6 in DMF containing K2CO3 to give benzhydrylcarbamoylmethylpiperazine II which prolonged survival of mice in a 4% O environment by 93% at 30 mg/kg i.p.

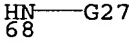
MSTR 1



G1 = 36-2 39-5



G9 = 68



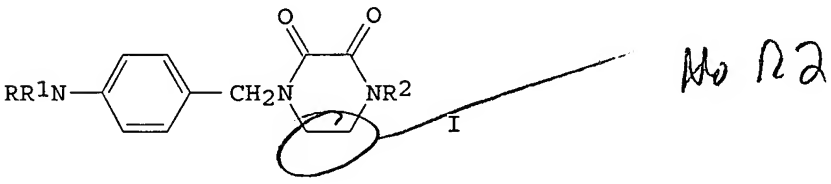
G27 = CH2Ph

G16+G17= O
G18+G19= O
Generic group attributes: 35 <containing 1-6 C>
Derivative: and pharmaceutically acceptable salts
Patent location: claim 1

L13 ANSWER 2 OF 2 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 101:151887 MARPAT
TITLE: 1-(4-Aminobenzyl)-2,3-dioxopiperazine derivatives and salts
INVENTOR(S): Hori, Takako; Yoshida, Chosaku; Kiba, Yasuo; Takeno, Ryuko; Nakano, Joji; Nitta, Jun; Kishimoto, Sumiko; Murakami, Shohachi; Tsuda, Hisatsugu; Saikawa, Isamu
PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd. , Japan
SOURCE: U.S., 13 pp. Cont.-in-part of U.S. Ser. No. 169,457.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4459407	A	19840710	US 1982-345055	19820202
JP 56018969	A2	19810223	JP 1979-93234	19790724
JP 05057272	B4	19930823		
US 4436921	A	19840313	US 1980-169457	19800716
JP 57140783	A2	19820831	JP 1981-15837	19810206
JP 63066319	B4	19881220		
US 4460774	A	19840717	US 1982-348271	19820212
US 4477666	A	19841016	US 1982-348272	19820212
US 4448963	A	19840515	US 1982-351257	19820222
US 4477664	A	19841016	US 1982-351256	19820222
PRIORITY APPLN. INFO.:			JP 1979-93234	19790724
			US 1980-169457	19800716
			JP 1981-15837	19810206

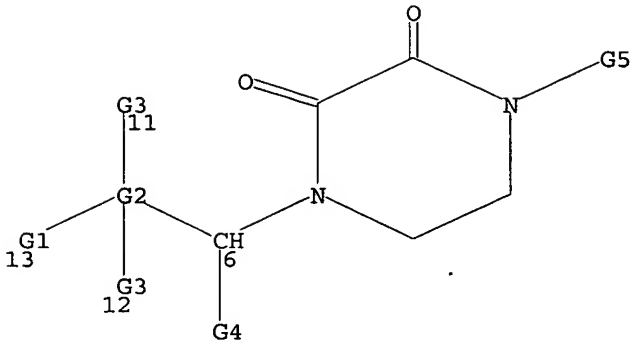
OTHER SOURCE(S): CASREACT 101:151887
GI



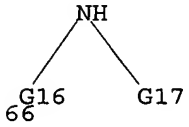
No R2

AB The carcinostatic title compds. I (R = pyrimidinyl, R1 = (un)substituted C1-8 alkyl; R2 = C1-8 alkyl, aralkyl) were prepared Thus, 1-(4-ethylaminobenzyl)-4-hexyldioxopiperazine was treated with 2-bromopyrimidine to give I (R = 2-pyrimidinyl, R1 = Et, R2 = hexyl). At 110 mg/kg I (R = 2-pyrinidinyl, R1 = MeOCH2, R2 = benzyl) increased the mean survival days of mice with inoculated L-1210 leukemia cells by a test group/control group ratio of 177%.

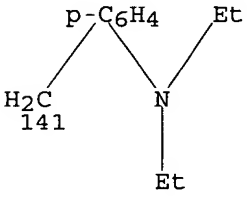
MSTR 1



G5 = 66



G16 = CH2CH2
G17 = 141



Patent location: claims
Note: record may include structures from disclosure